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Title: Numerical Diffusion (Mixing) of Material in Numerical Simulations of Hydrodynamics

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Numerical Diffusion (Mixing) of Material in Numerical Simulations for Hydrodynamics

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Michael Steinkamp, Jim Ferguson, Joann Campbell, Chris Werner

Abstract

It is often assumed that a material interface between two materials is spread over a few numerical cells in numerical simulations for hydrodynamics. Also, we have the impression that higher order methods introduce less numerical diffusion (mixing) of material. As we know one of the purposes of adaptive mesh refinement (AMR) is to resolve interfaces between materials, but we would like to know how effective AMR is to reduce numerical diffusion of material. We will present our investigation about numerical diffusion (mixing) of material in xRage. The result of the investigation indicates that the assumptions mentioned above are not always valid. In this talk, we will also demonstrate the effectiveness of numerical techniques to reduce numerical diffusion of material, including contact discontinuity steepening, isotropic interface steepening, max interface steepening, material interface reconstruct.

Outlines

- Motivations
- Hydro Algorithms

  Split, unsplit, Riemann solver

  Interpolation, monotonicity condition

  Interface treatment: contact discontinuity steepening, isotropic interface steepening, max interface steepening, interface reconstruction
- Numerical Examples to show numerical mixing
- Conclusions

Motivations

- Material mixing is extremely important for many problems.
- Numerical mixing is difficult to separate from physics mixing in calculations.
- Are Eulerian codes more diffusive than Lagrangian codes ?
- How many cells is a material interface spread over ?
- Does AMR (alone) effectively reduce numerical mixing ?
- Higher order method = less numerical mixing ?

    discontinuity/interface *vs* order of accuracy
- How could we reduce numerical mixing if VoF not applicable.

Euler Equations

$$\frac{\partial \rho}{\partial t} = \bigtriangledown \cdot \rho \mathbf{u} = 0,$$

$$\rho(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \bigtriangledown)\mathbf{u} = - \bigtriangledown p,$$

$$\frac{\partial}{\partial t}[\rho(\frac{1}{2}\mathbf{u}^2 + \epsilon)] = - \bigtriangledown \cdot [\rho \mathbf{u}(\frac{1}{2}\mathbf{u}^2 + \epsilon + \frac{1}{\rho}p)].$$

Multi-materials

$$\rho = \sum_i v_i \rho_i,$$

$$p = \sum_i v_i p_i,$$

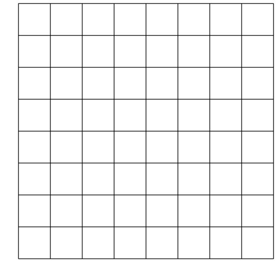
$$\varepsilon = \frac{1}{\rho}\sum v_i \rho_i \varepsilon_i.$$

Euler Equations

$$\frac{\partial U}{\partial t} + \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z} = 0. \qquad \mathbf{U} \equiv \begin{pmatrix} \rho \\ \rho u_x \\ \rho u_y \\ \rho u_z \\ \rho\epsilon \end{pmatrix}$$

$$F_x \equiv \begin{pmatrix} \rho u_x \\ \rho u_x^2 + p \\ \rho u_x u_y \\ \rho u_x u_z \\ u_x(\rho\epsilon + p) \end{pmatrix} \quad F_y \equiv \begin{pmatrix} \rho u_y \\ \rho u_y u_x \\ \rho u_y^2 + p \\ \rho u_y u_z \\ u_y(\rho\epsilon + p) \end{pmatrix} \quad F_z \equiv \begin{pmatrix} \rho u_z \\ \rho u_z u_x \\ \rho u_z u_y \\ \rho u_z^2 + p \\ u_z(\rho\epsilon + p) \end{pmatrix}$$

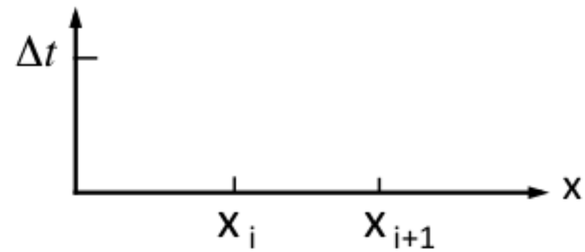
Dimensionally Split Approach



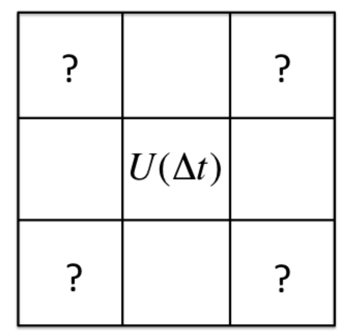
$$\frac{\partial U}{\partial t} + \frac{\partial F_x}{\partial x} = 0$$

$$U_{i,j,k}(\triangle t) = U_{i,j,k}(0) + \frac{\triangle t}{\triangle x_i}[\bar{F}_{xj,k}(x_i) - \bar{F}_{xj,k}(x_{i+1})]$$

$$U_i(\Delta t) \equiv \frac{1}{\Delta x}\int_{x_i}^{x_{i+1}} U(\Delta t, x)\,dx.$$



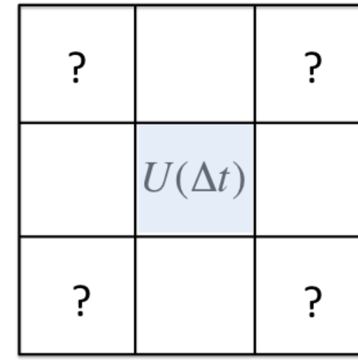
$$\overline{F_x}(x_i) \equiv \frac{1}{\Delta t}\int_0^{\Delta t} F(t, x_i)\,dt.$$



Corner- and edge-coupling

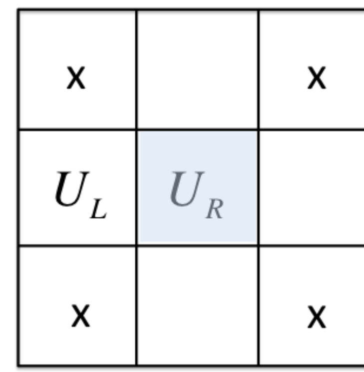
Second order accurate if each pass is. (Strang, 1968)

Unsplit Approach

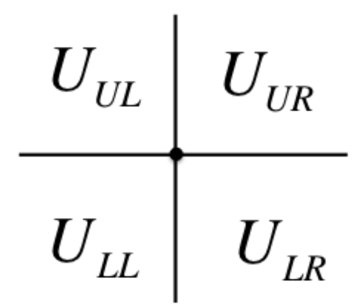


$$\frac{\partial U}{\partial t} + \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z} = 0.$$

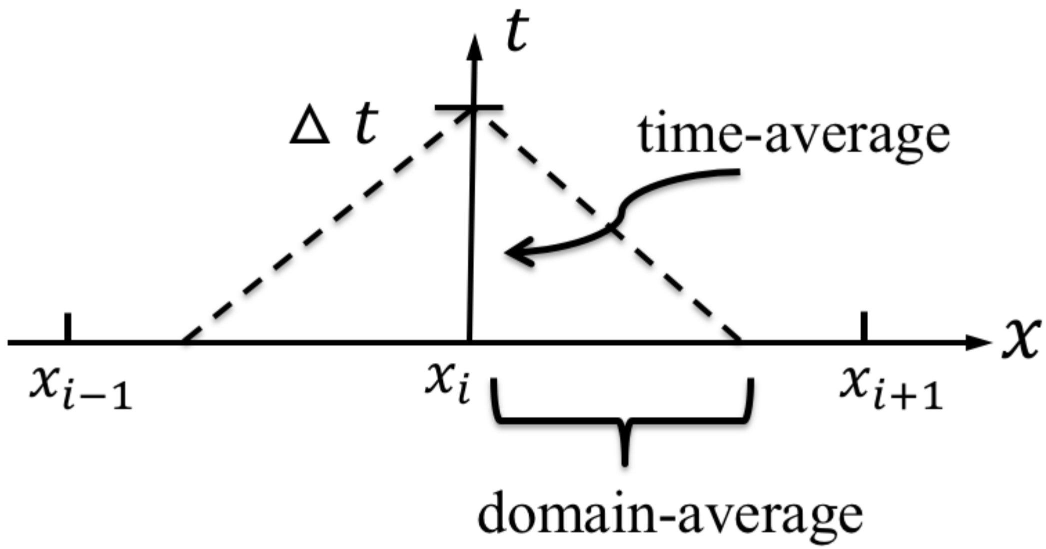
$$\begin{aligned} U_{i,j,k}(\triangle t) = U_{i,j,k}(0) &+ \frac{\triangle t}{\triangle x_i}[\bar{F}_{xj,k}(x_i) - \bar{F}_{xj,k}(x_{i+1})] \\ &+ \frac{\triangle t}{\triangle y_j}[\bar{F}_{yi,k}(y_j) - \bar{F}_{yi,k}(y_{j+1})] \\ &+ \frac{\triangle t}{\triangle z_k}[\bar{F}_{zi,j}(z_k) - \bar{F}_{zi,j}(z_{k+1})] \end{aligned}$$



- Flux calculated simultaneously
- In general, fluxes depend on corner- and edge-cells.
- One approach: no corner- and edge-coupling
- Other approach: including corner cells in flux, ex, Riemann problem at grid points

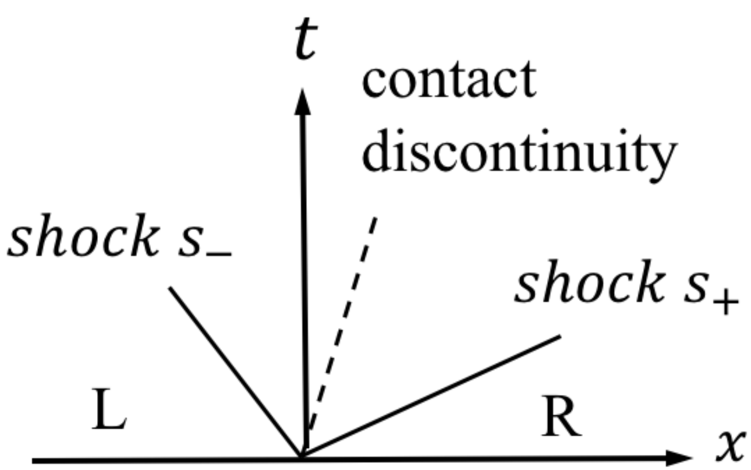


from domain-average to time-average

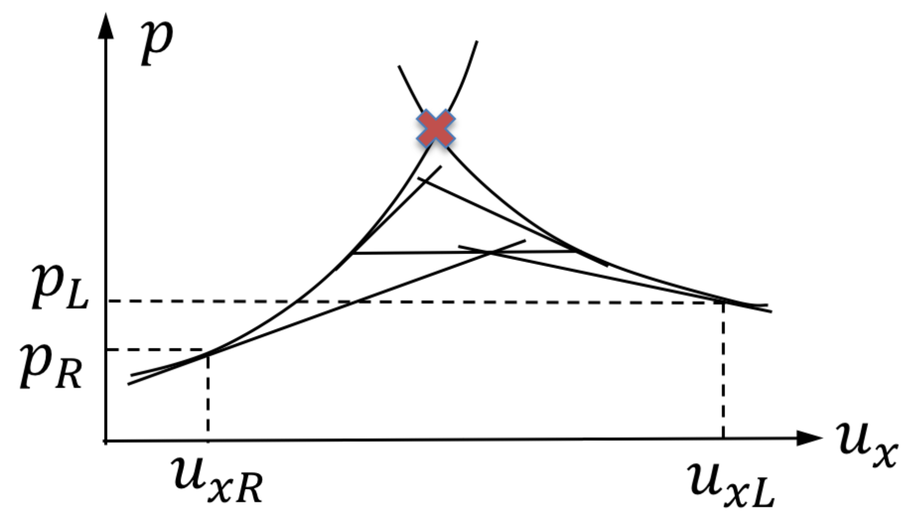


$$\overline{F_x}(x_i) \equiv \frac{1}{\Delta t}\int_0^{\Delta t} F(t, x_i)\,dt.$$

Calculation of the time averaged velocity $\bar{u}_x$: 1D Riemann problem & solvers



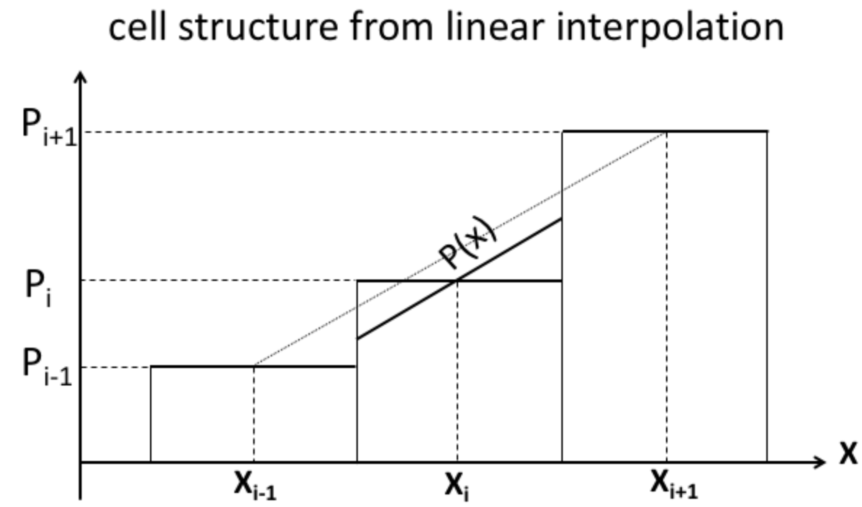
1D Riemann problem & solutions



1D linear and nonlinear Riemann solver

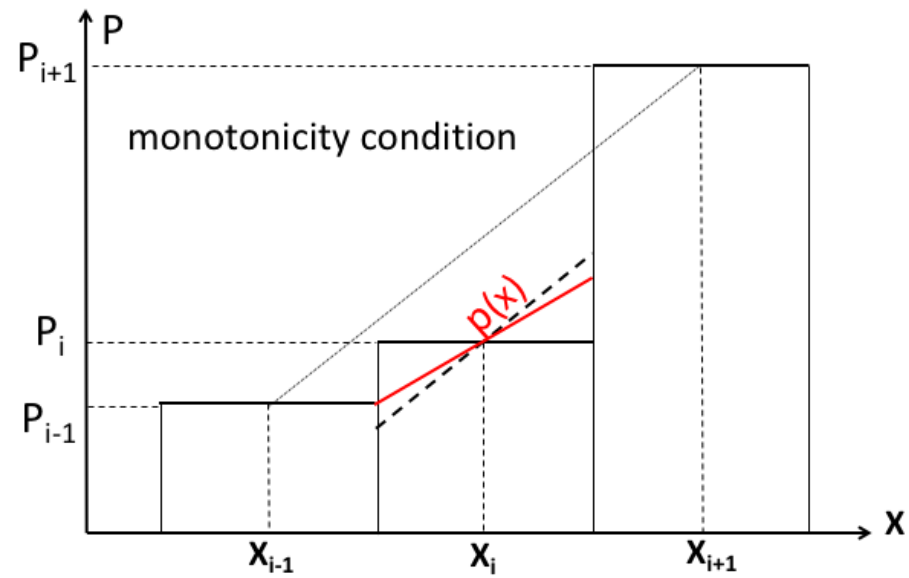
- Interpolation

purpose:
realize **2^{nd} order accurate** in space



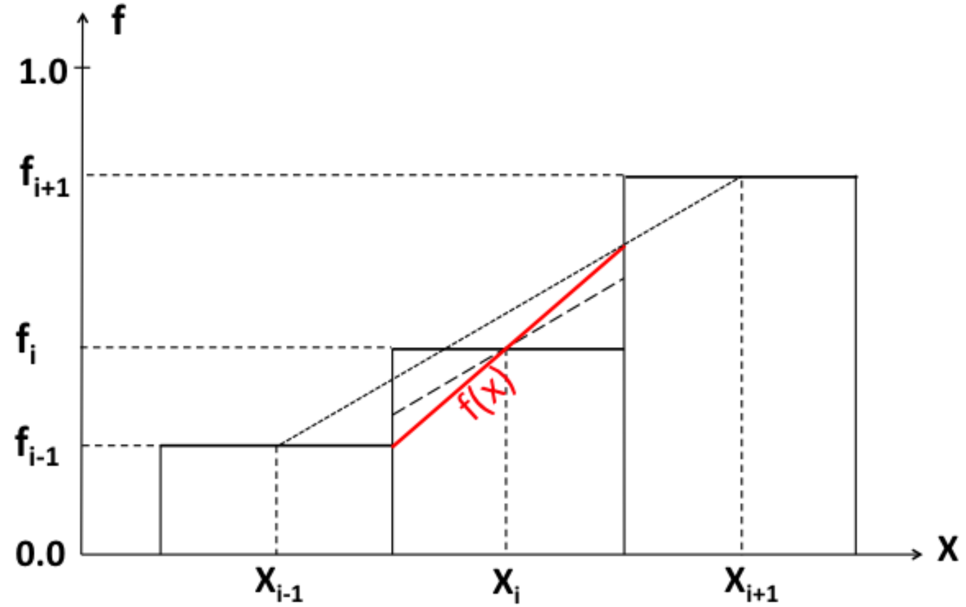
- Brian Van Leer's monotonicity condition

purpose:
Removed under- & over-shoot
fluctuation near shocks



- Contact Discontinuity Steepening

purpose:
reduce numerical diffusion of material near interface

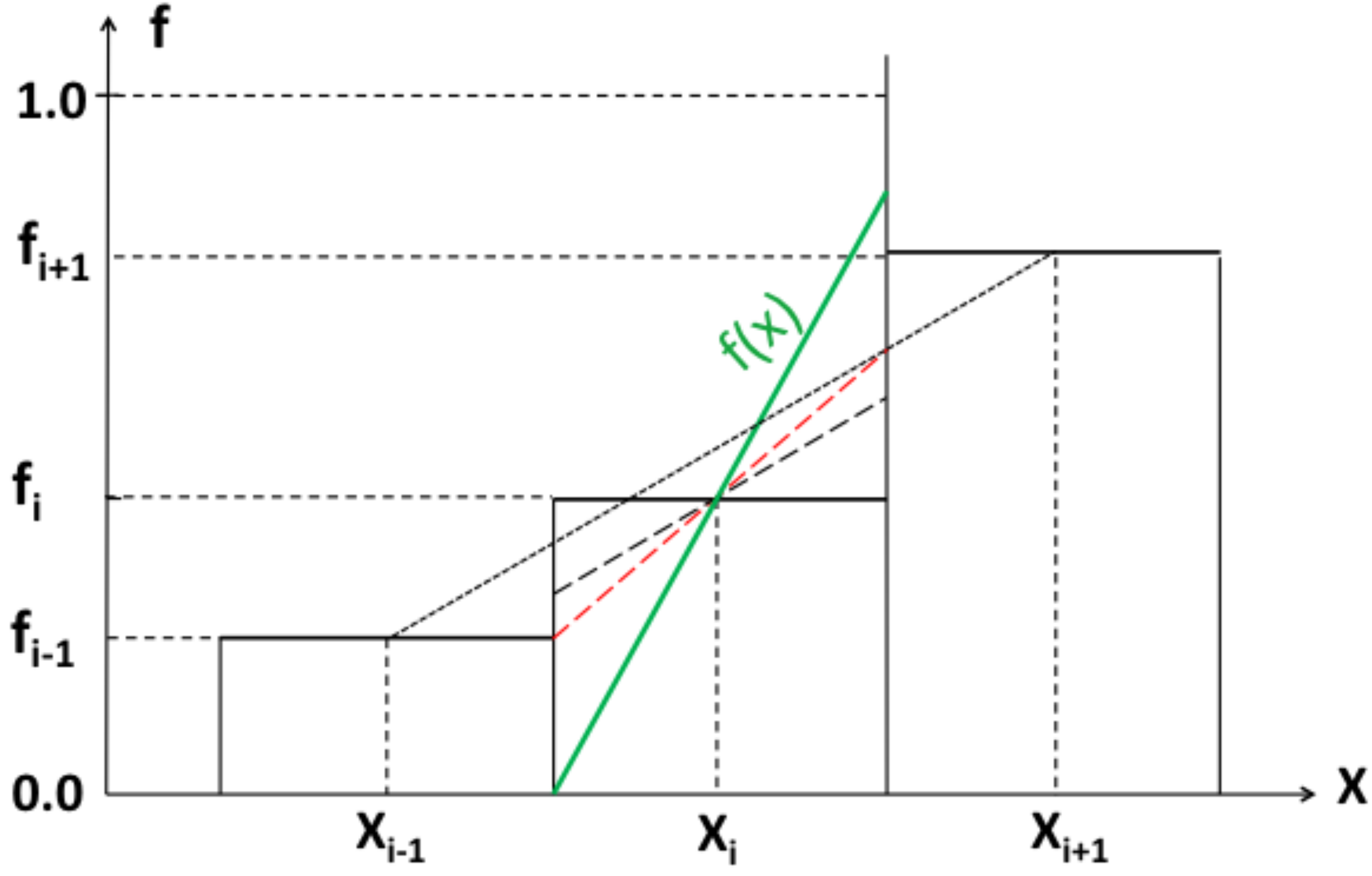


- Isotropic Interface Steepening

Purpose:
Keep isotropic feature of material interfaces

- max interface steepening

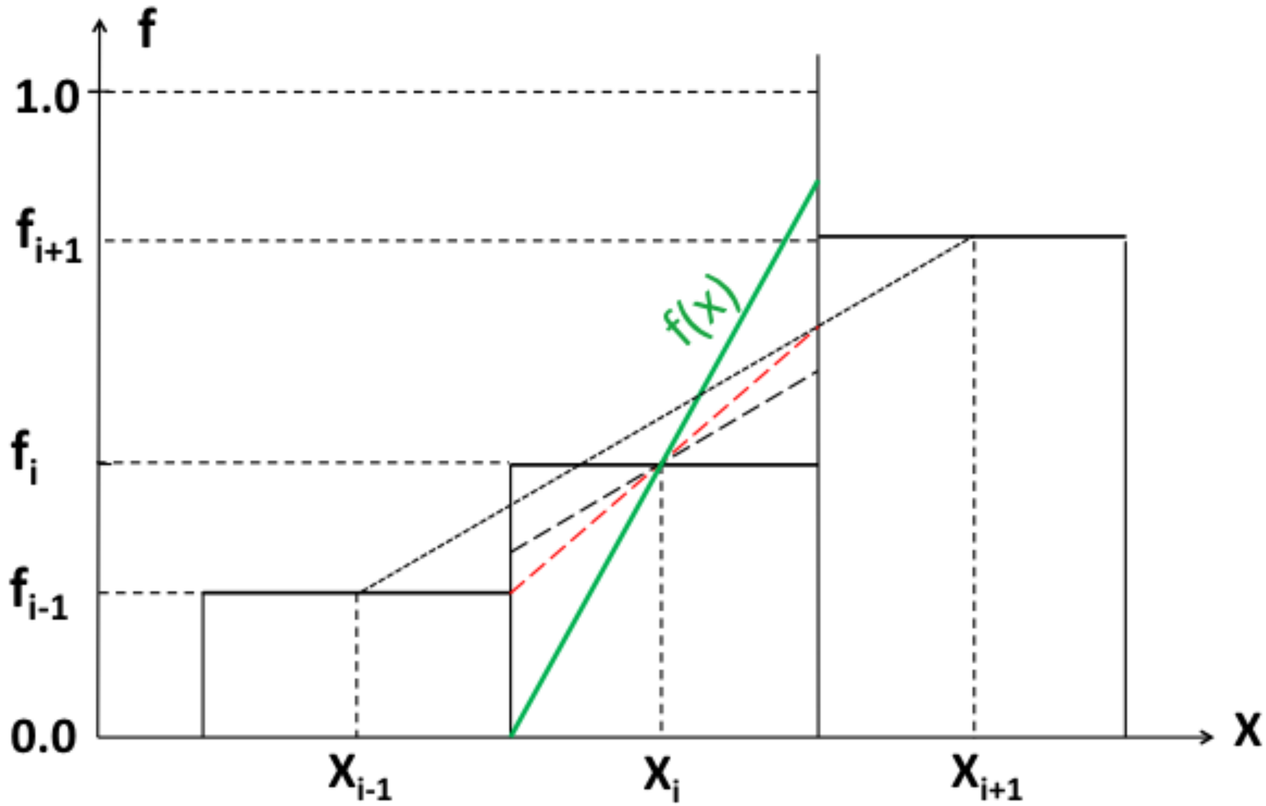
purpose:
Further reduce numerical diffusion near material interfaces



max interface steepening

vs

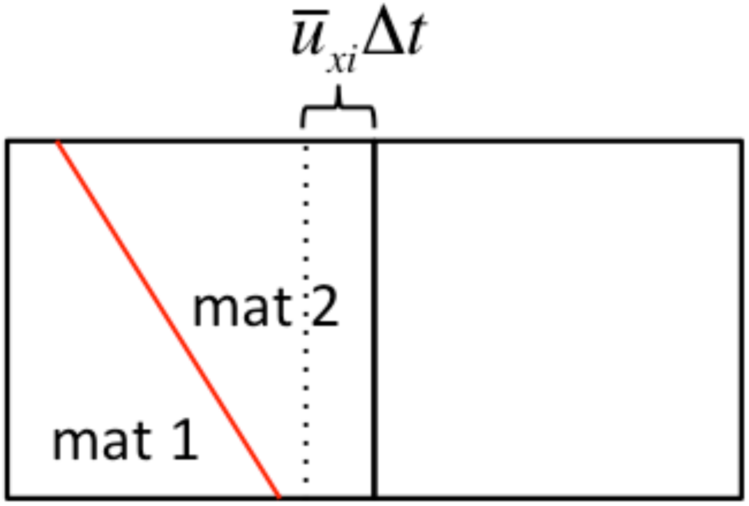
normal interface steepening

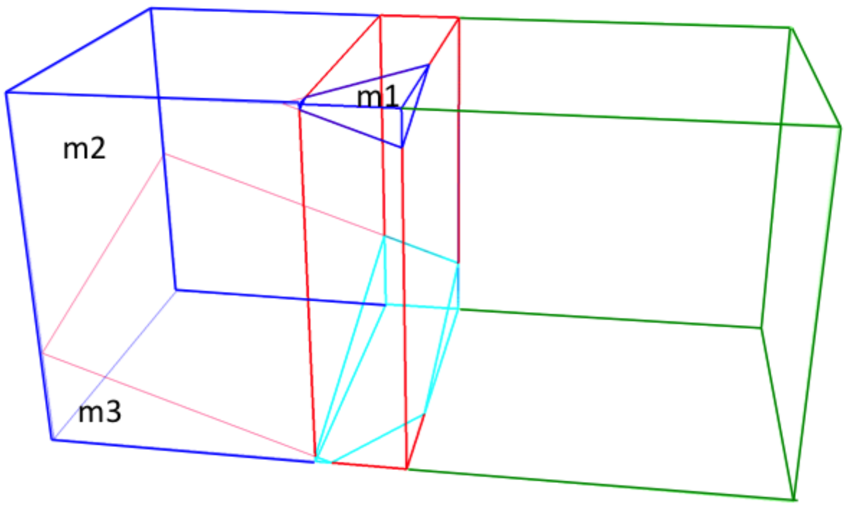


Reconstruction of Material Interface

Why Interface Reconstruction

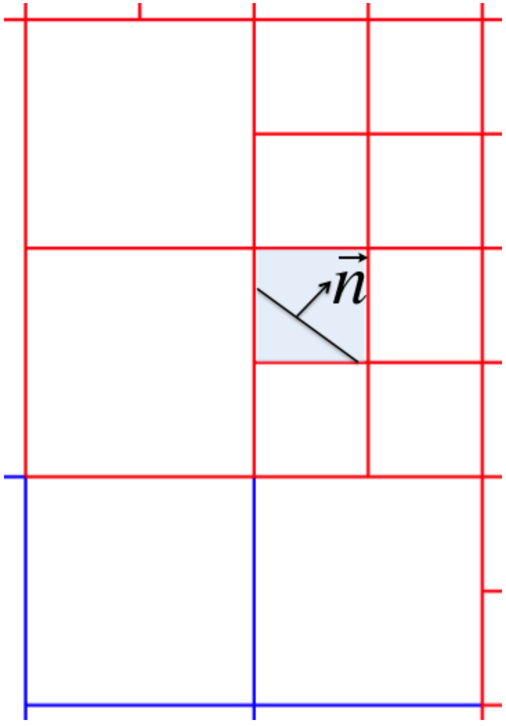
One of many reasons: reduce numerical mixing in hydro





Linear Material Interface: $\vec{n}\cdot\vec{r}=c$

- Step 1: Normal direction of interface



$$\vec{v}_m = \sum_{k=1}^{Nb} \frac{1}{d_k} (\vec{r}_k - \vec{r}_0)(f_{mk} - f_{m0})$$

$$p_m \equiv |\vec{v}_m|^2 \sqrt{f_m}$$

The $\vec{v}_m$ with the large p_m will be used for the normal direction of the interface

$$\vec{n} \equiv \vec{v}_{m0} / |\vec{v}_{m0}|$$

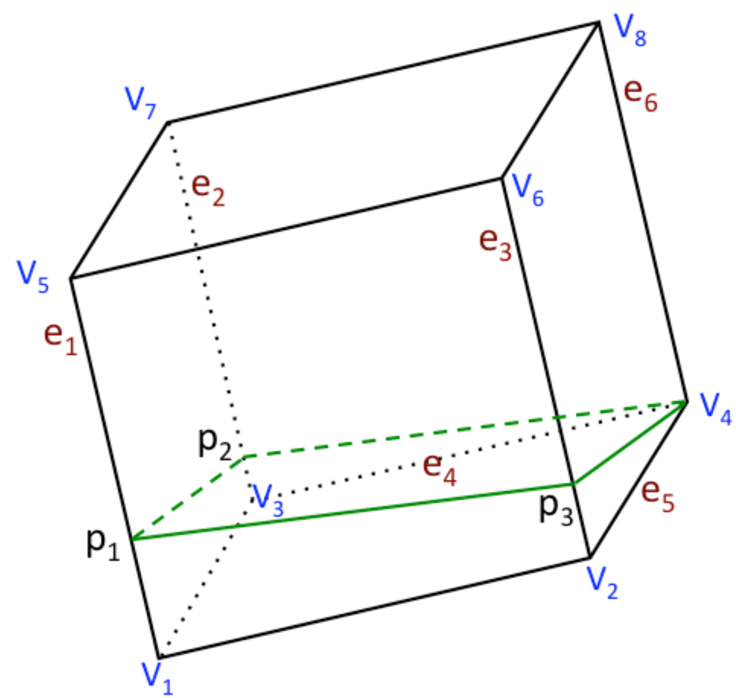
- Step 2: rotate polyhedron

Rotate the coordinate system so that the z-axis points to the normal direction

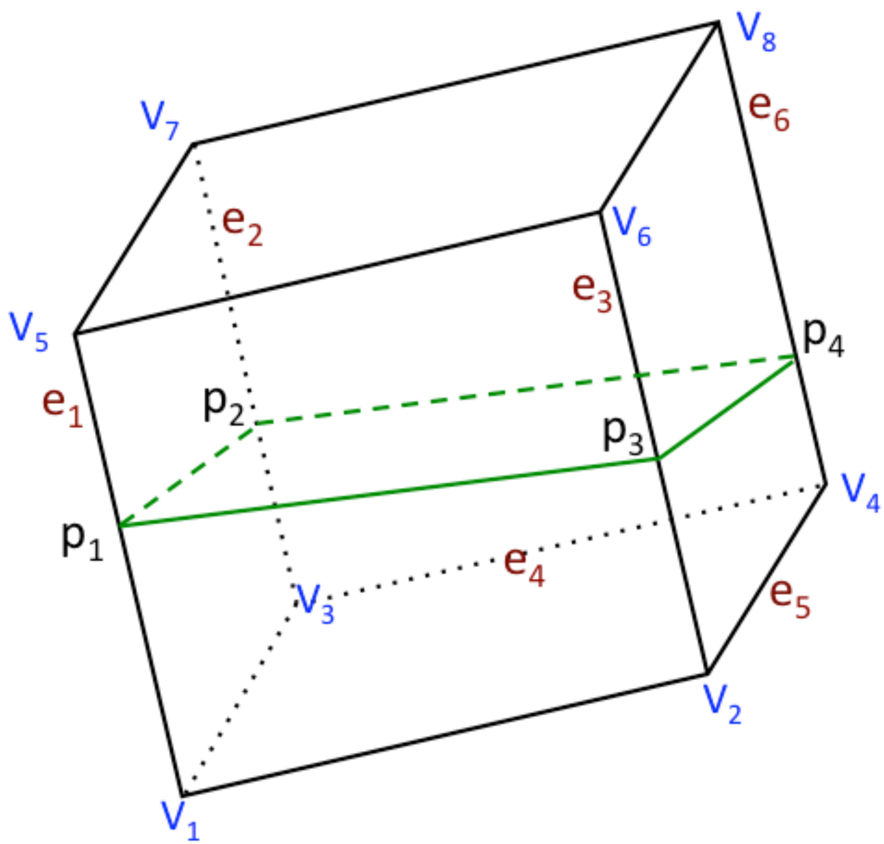
$$z = z_0$$

- Step 3: order nodes and find their associated volumes

Order the nodes of the polyhedron according to their z-values.
Find planes of intersection through nodes, and their associated volumes



- Step 4: Find the interface within the required accuracy



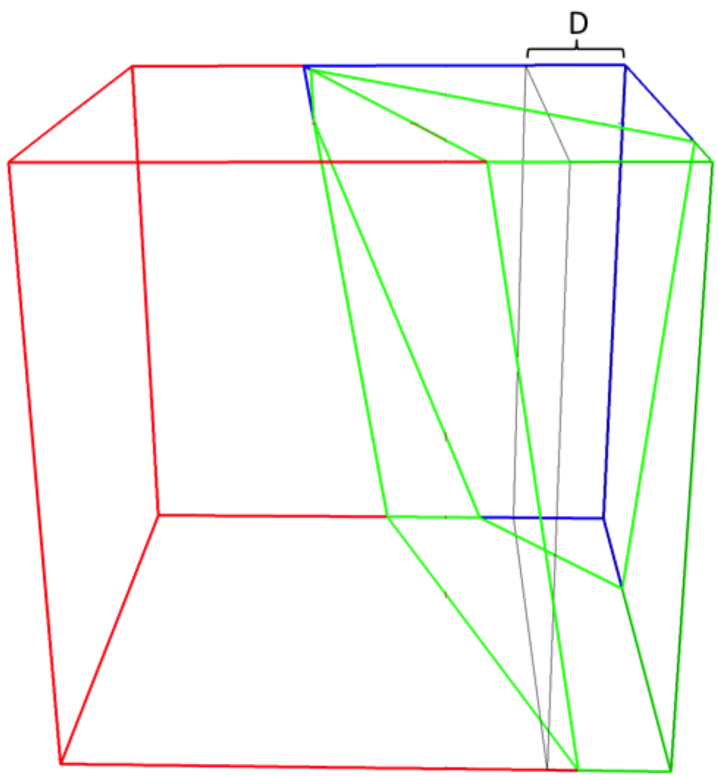
$$v_{i-1} < v < v_i$$

- Step 5: rotate back to the original coordinate system

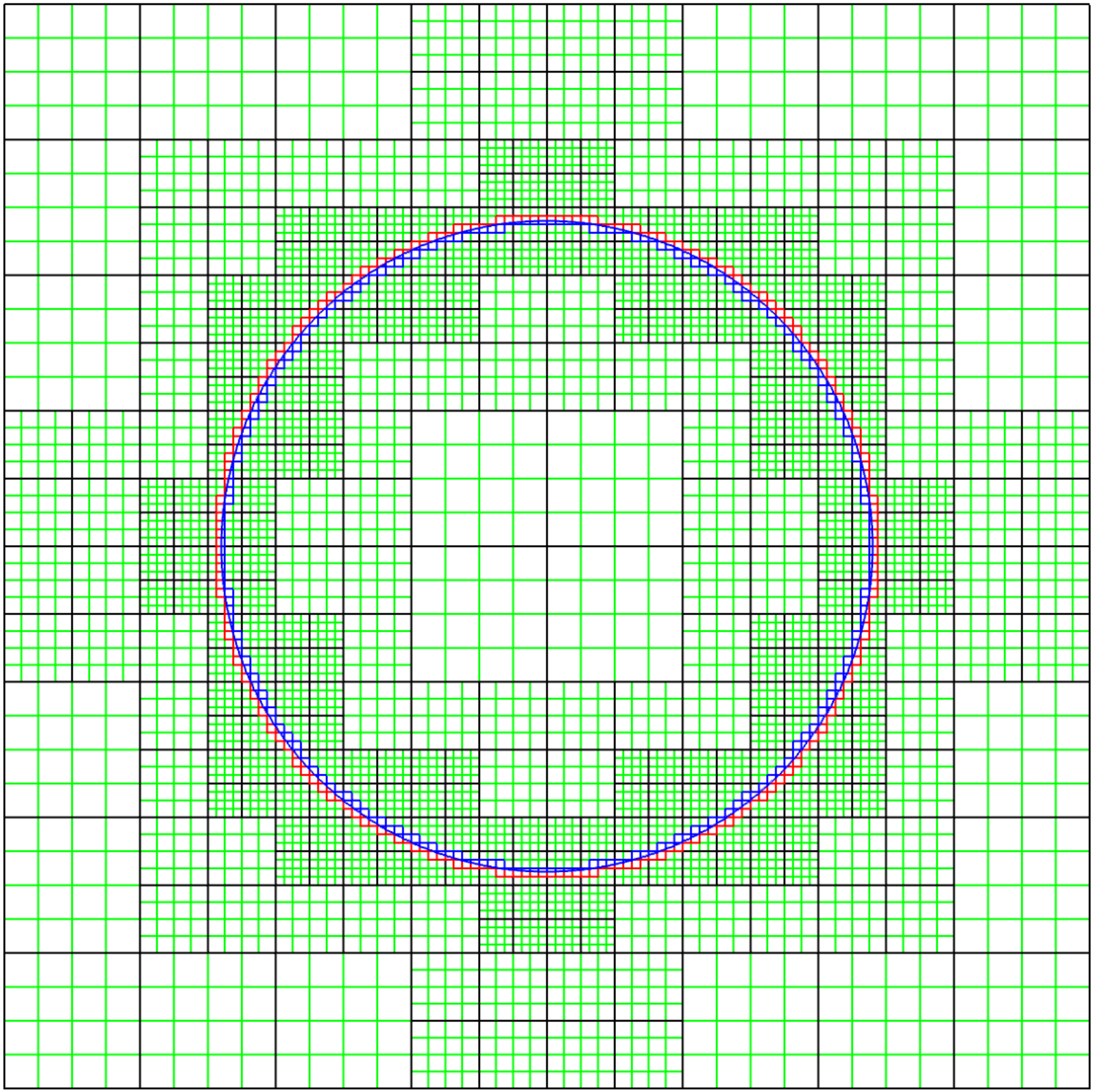
The same procedure works for 2D except for rotation.

More than two materials in a mixed cells

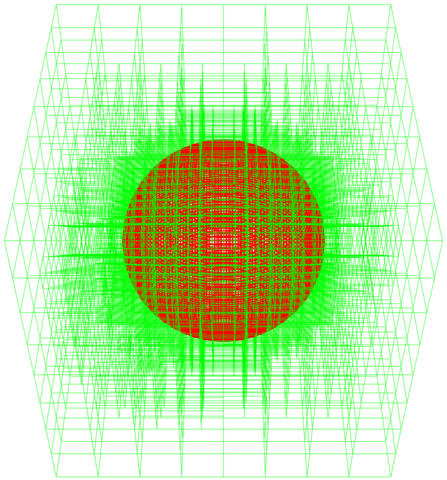
- Reduce a problem with M materials into (M-1) problems, each of which is considered a problem with only *two* materials.
- The polyhedron of each problem is the output of the previous problem.

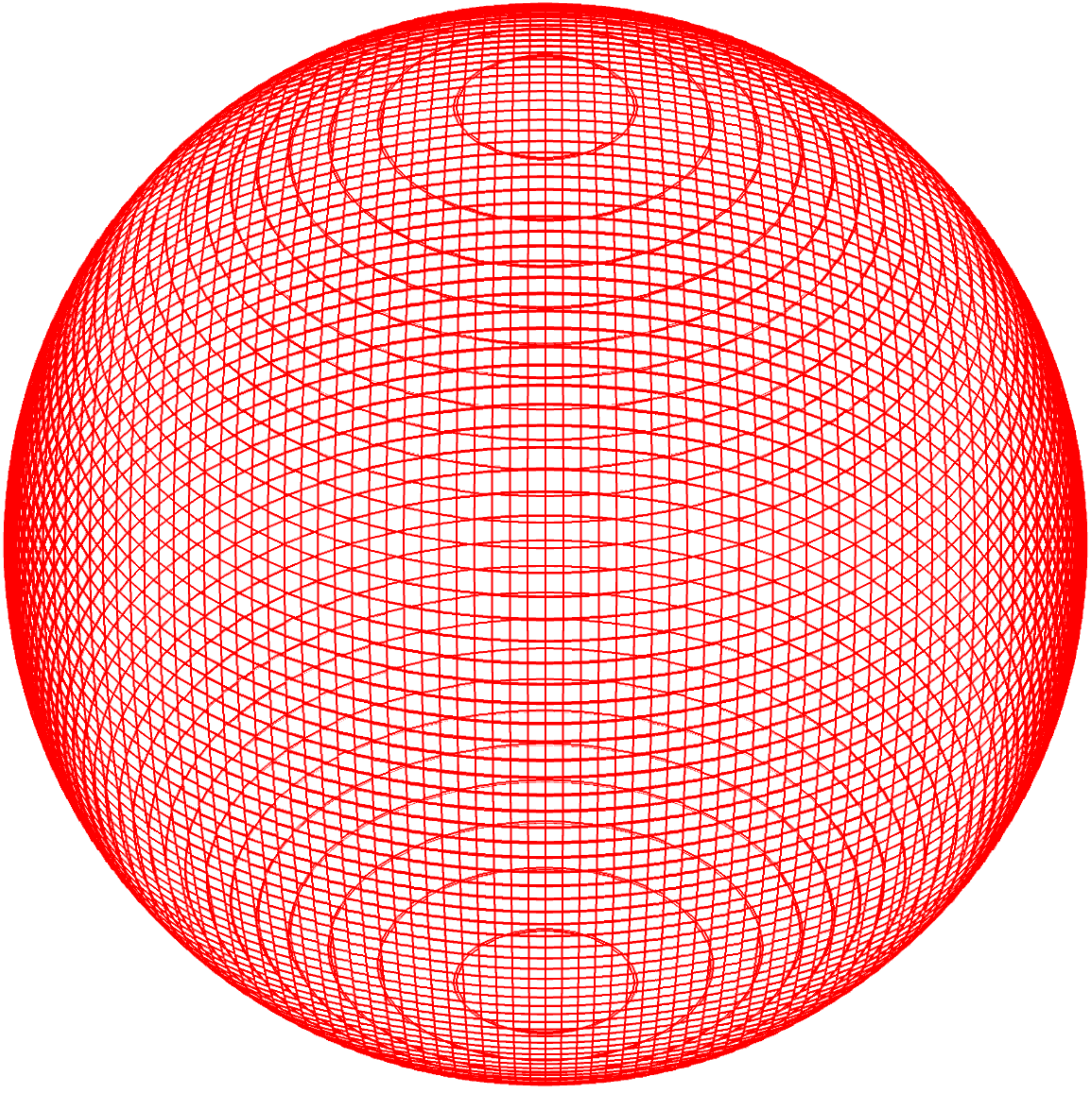


2D example of Reconstruction



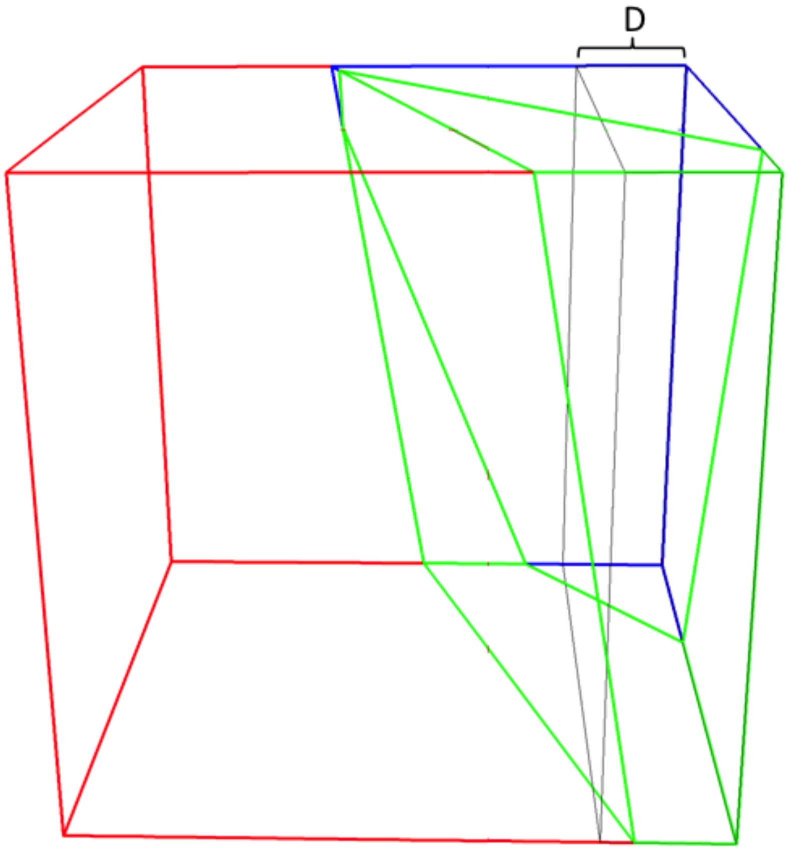
3D example of Reconstruction



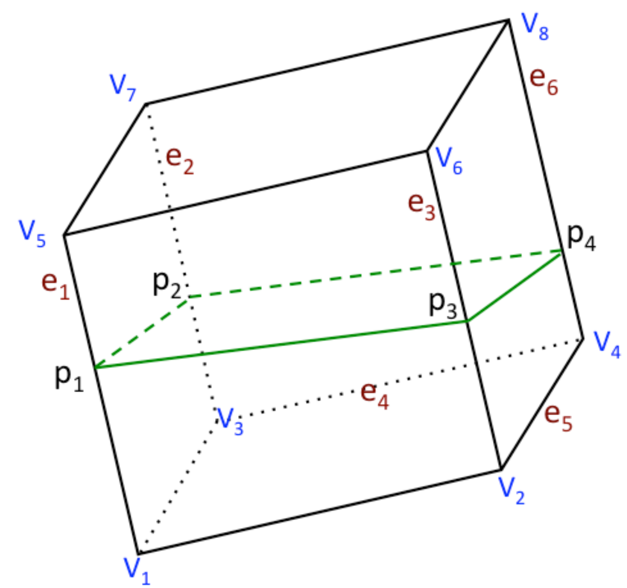


Applications of Interface Reconstruction

dimensionally split hydro

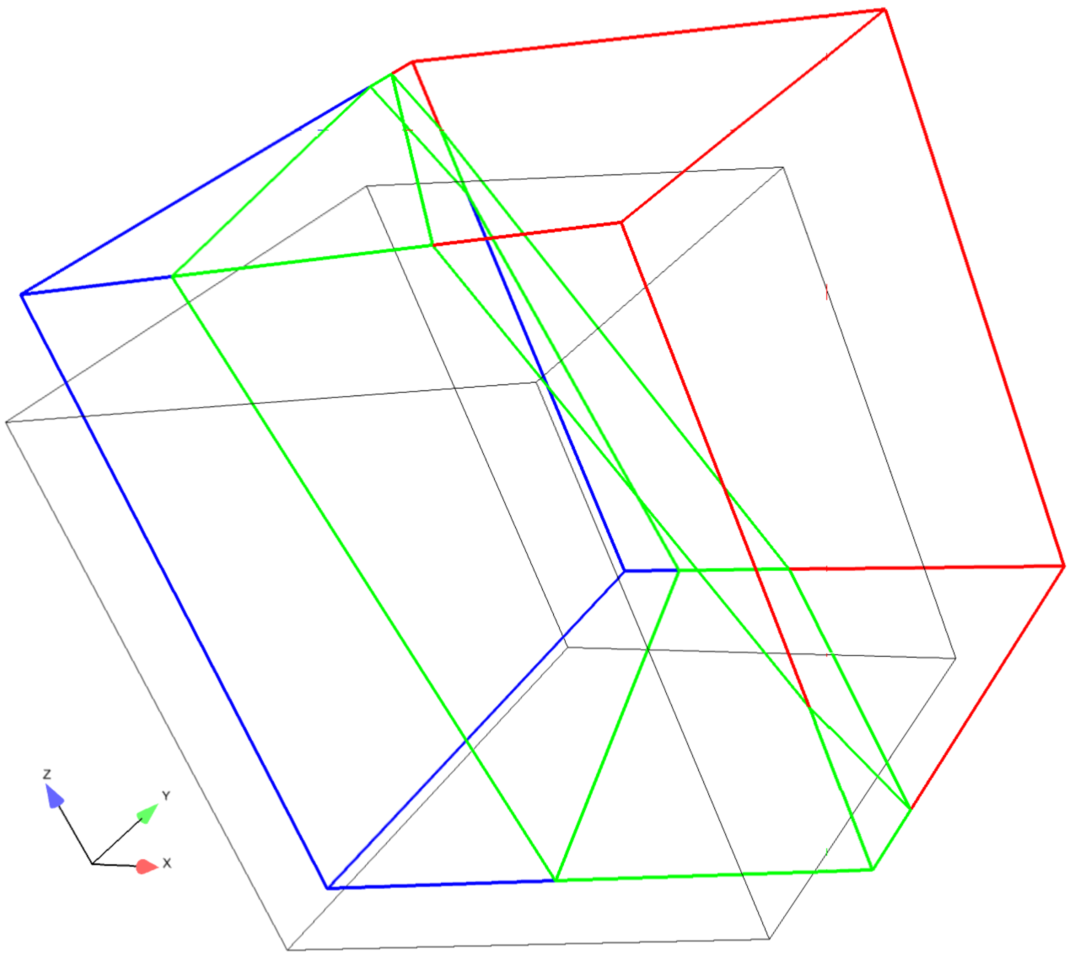


same code for intersecting a polyhedron by a plane



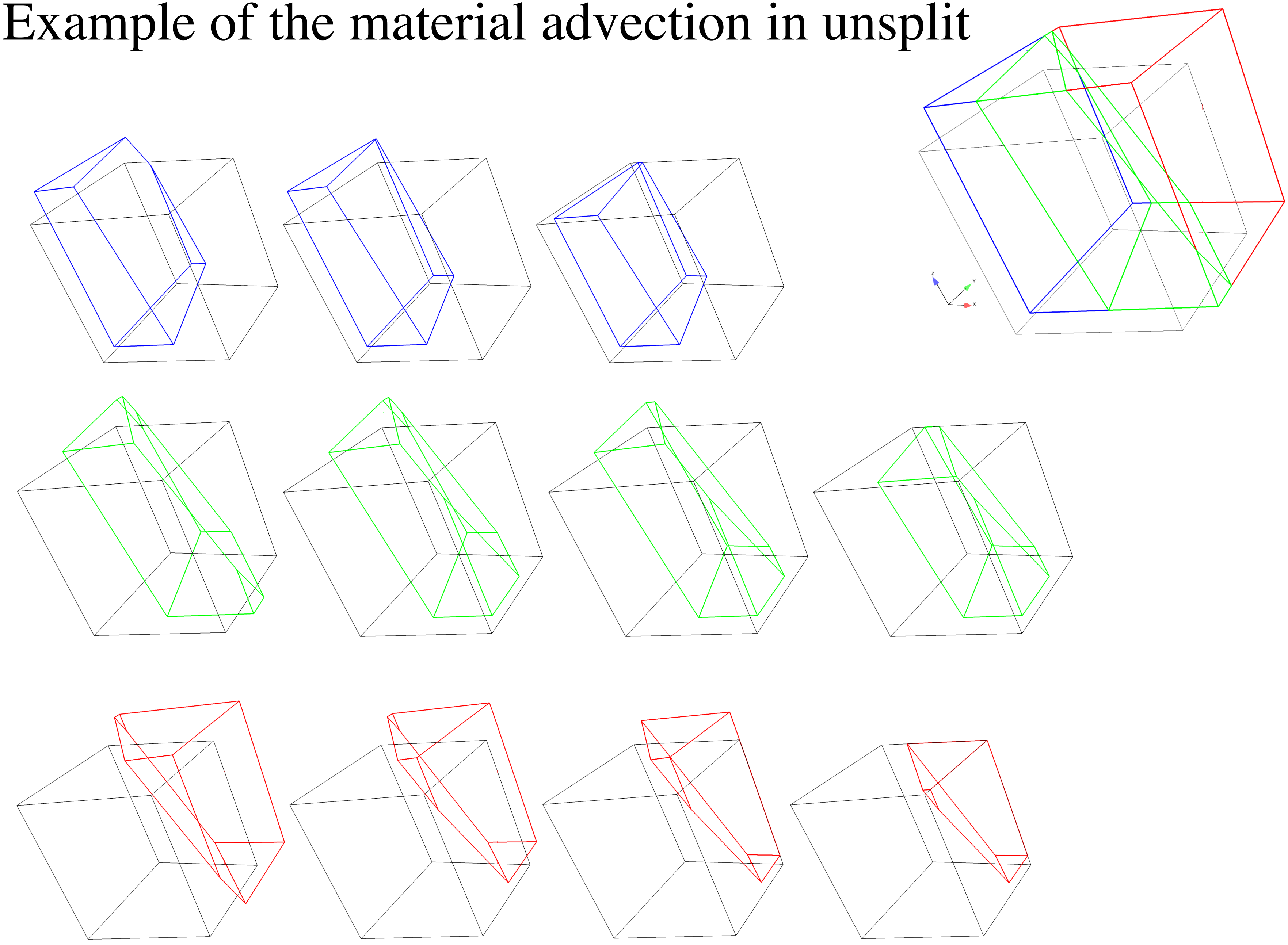
Applications of Interface Reconstruction

dimensionally unsplit hydro



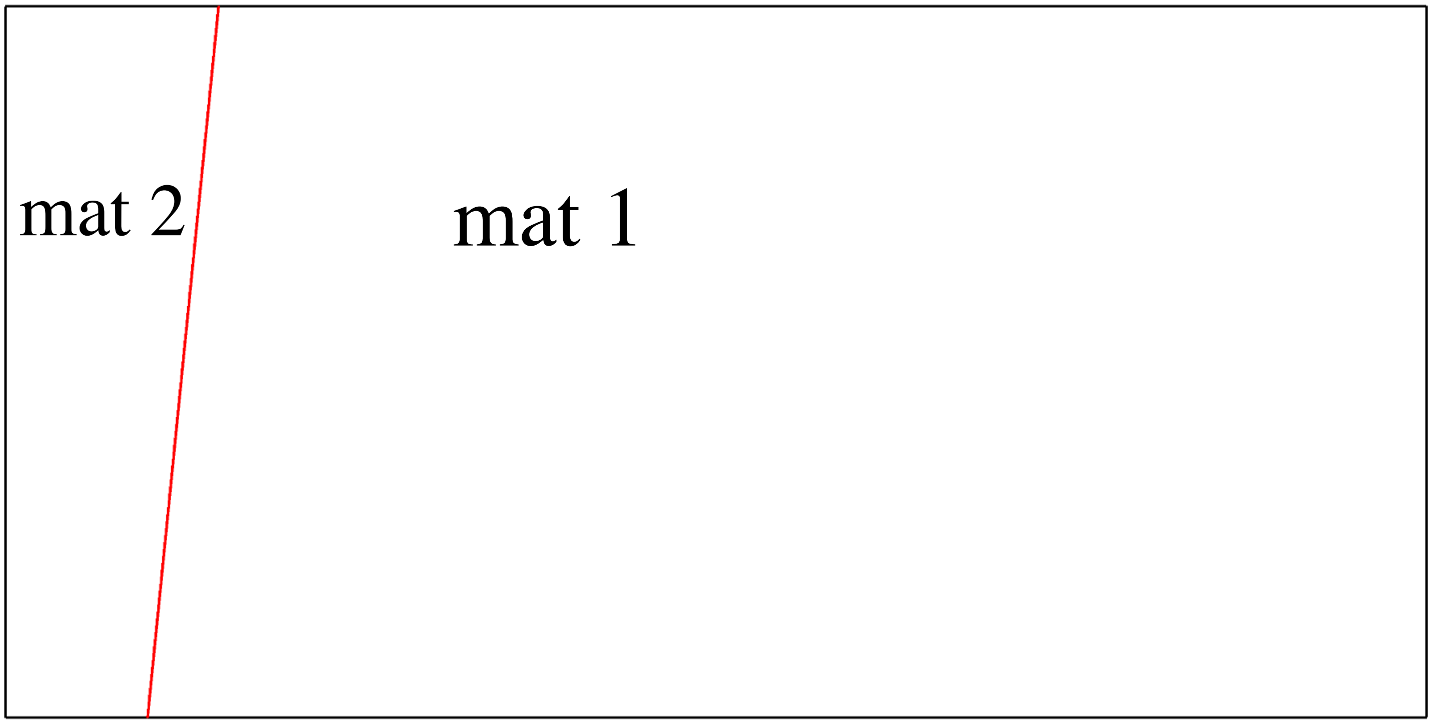
same by a plane code for intersecting a polyhedron

Example of the material advection in unsplit

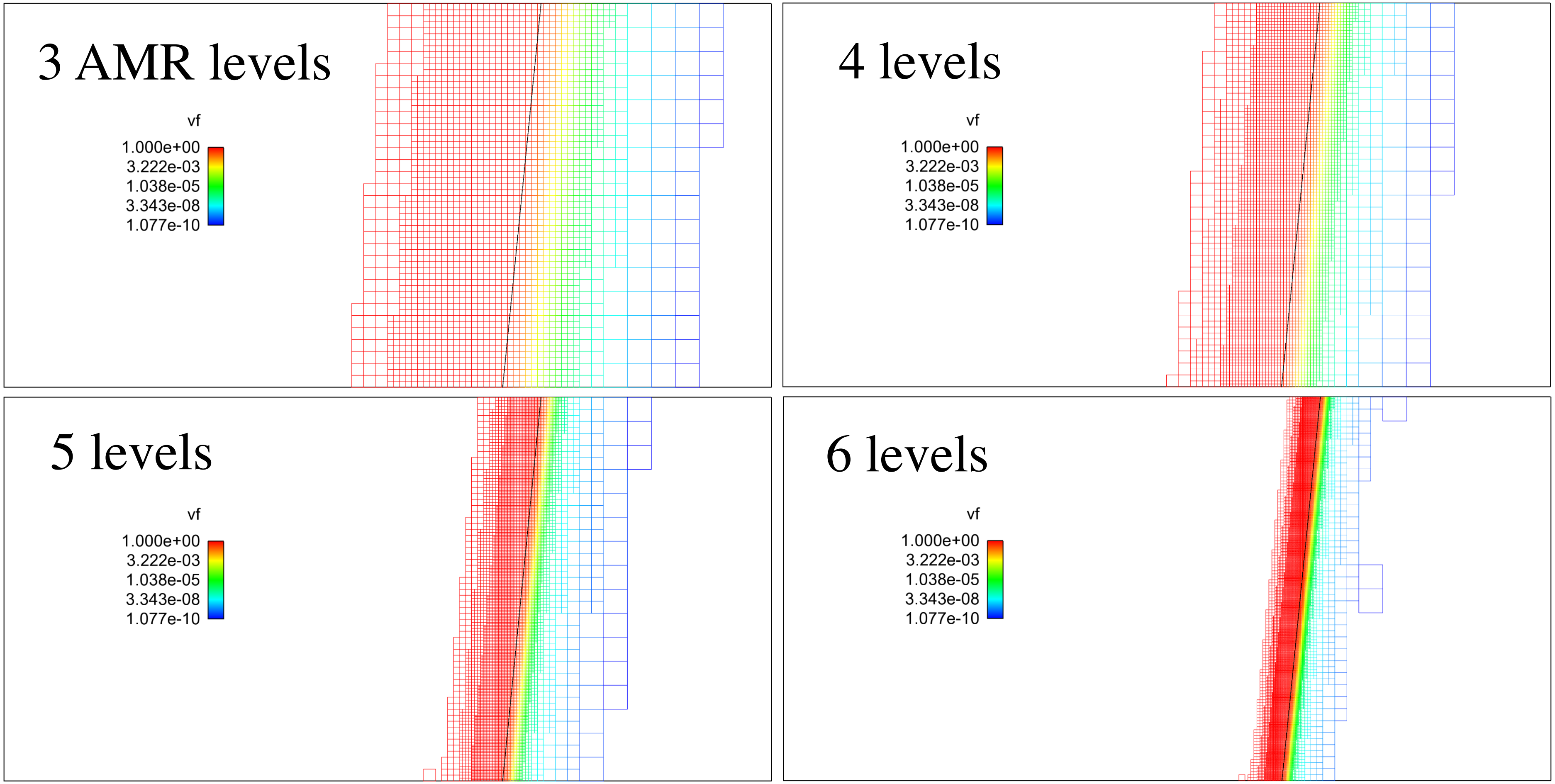


Examples of Numerical Mixing

Example 1 : Two materials with balanced pressure

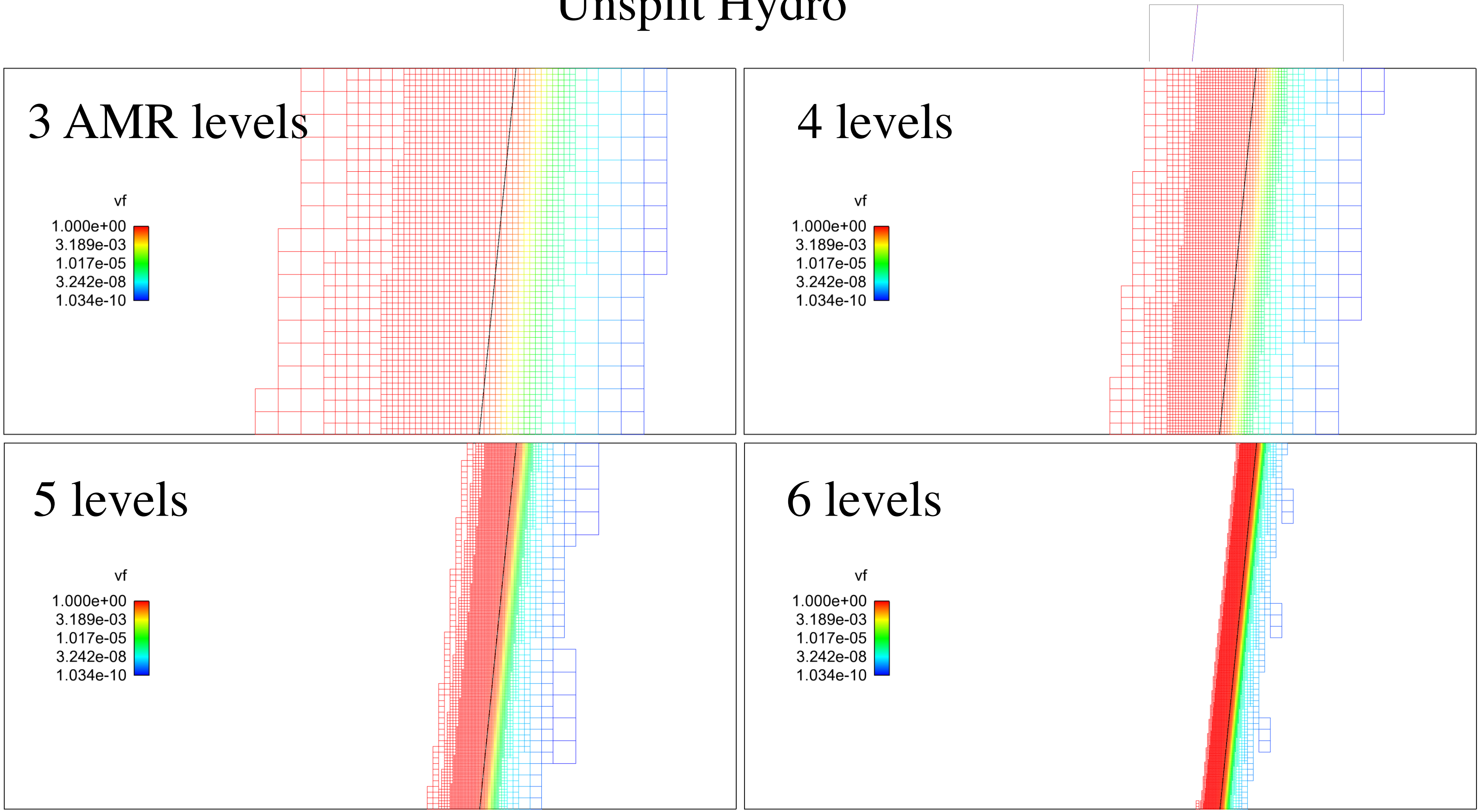


Default Hydro



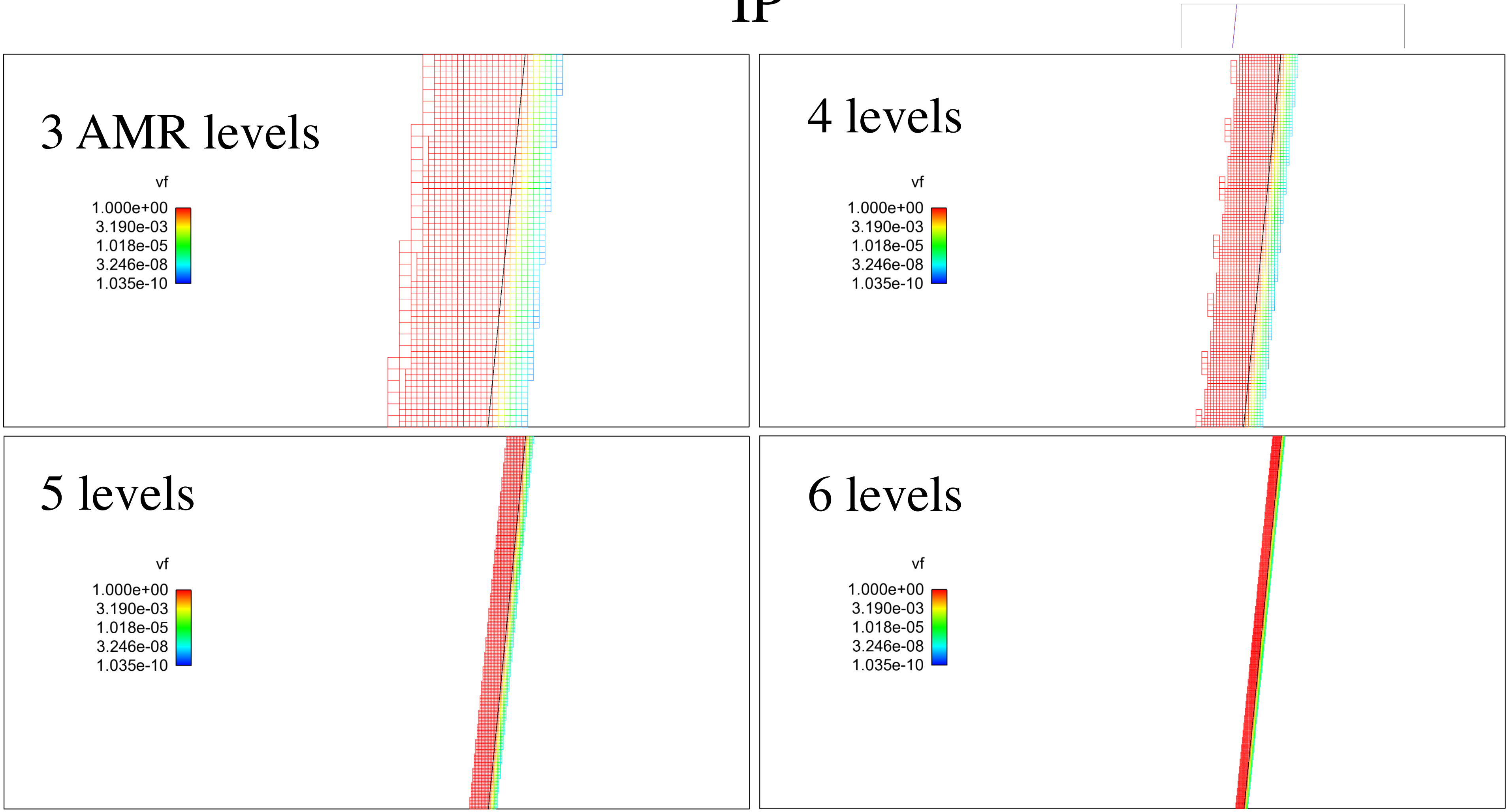
- The region of mixed cells decreases with AMR level, but not by factor 2 with each level.
- The numbers of mixed cells are roughly same, about 40 cells.
- This is the result of a method with 2[nd] order accuracy.

Unsplit Hydro



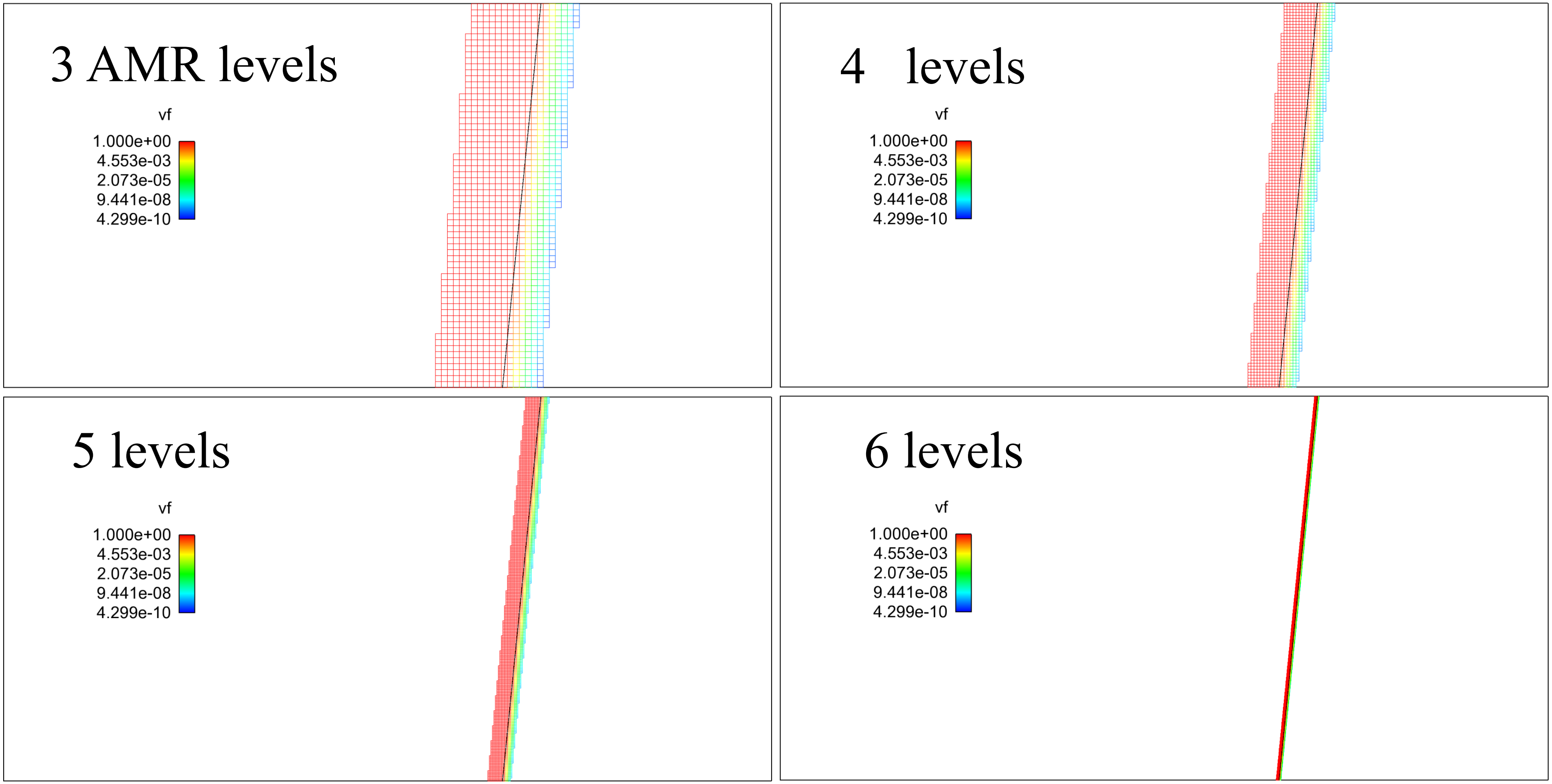
numerical mixing similar to split hydro

IP



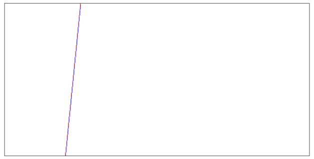
- The region of mixed cells decreases with AMR level, roughly by a factor 2 with each level.
- The number of mixed cells is reduced by a factor 2.
- This is the result of a method with the first order accuracy.

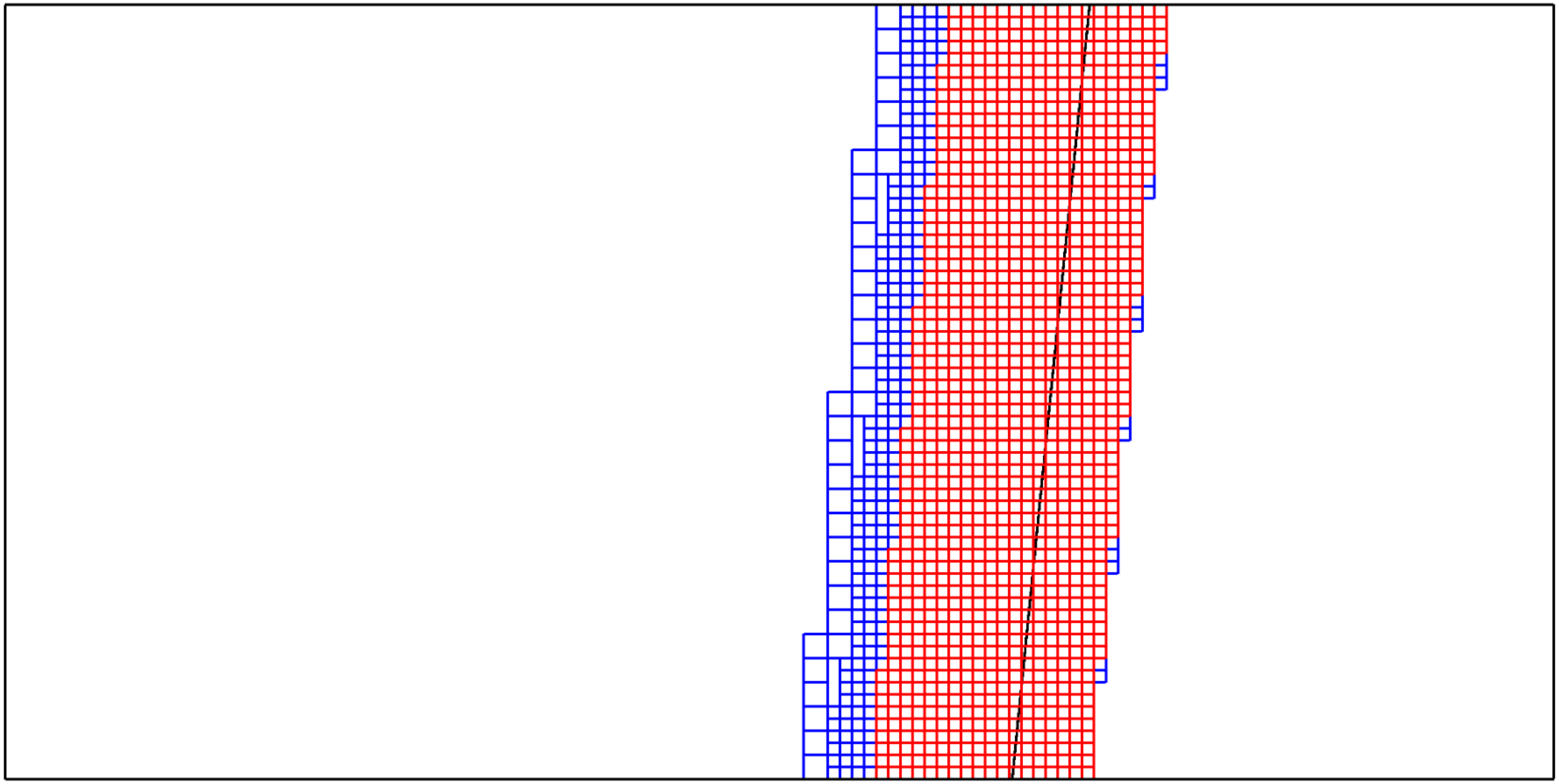
max_interface_steepening



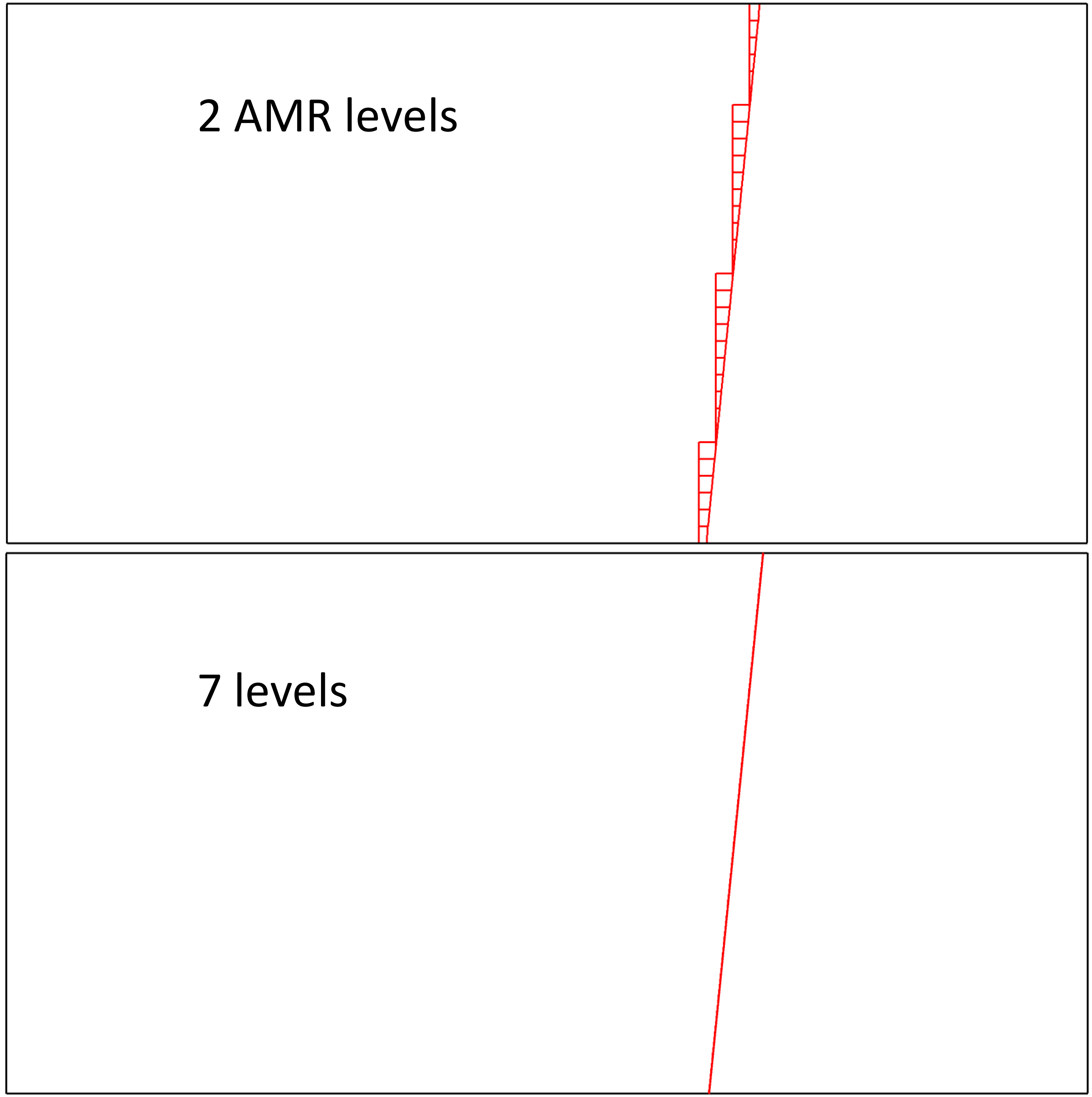
- Further reduced the number of mixed cells.

IP vs max_niterface_steepening



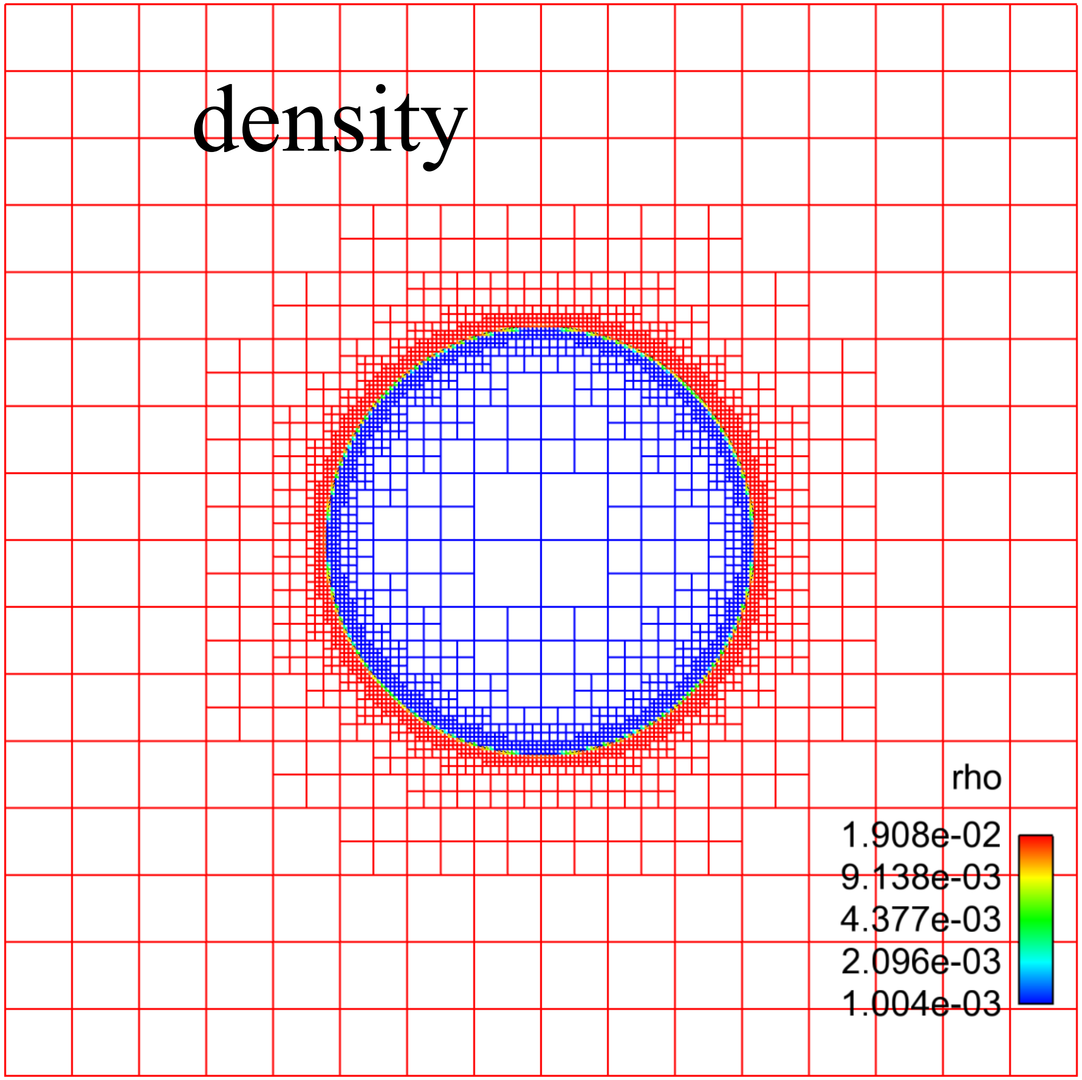


VoF



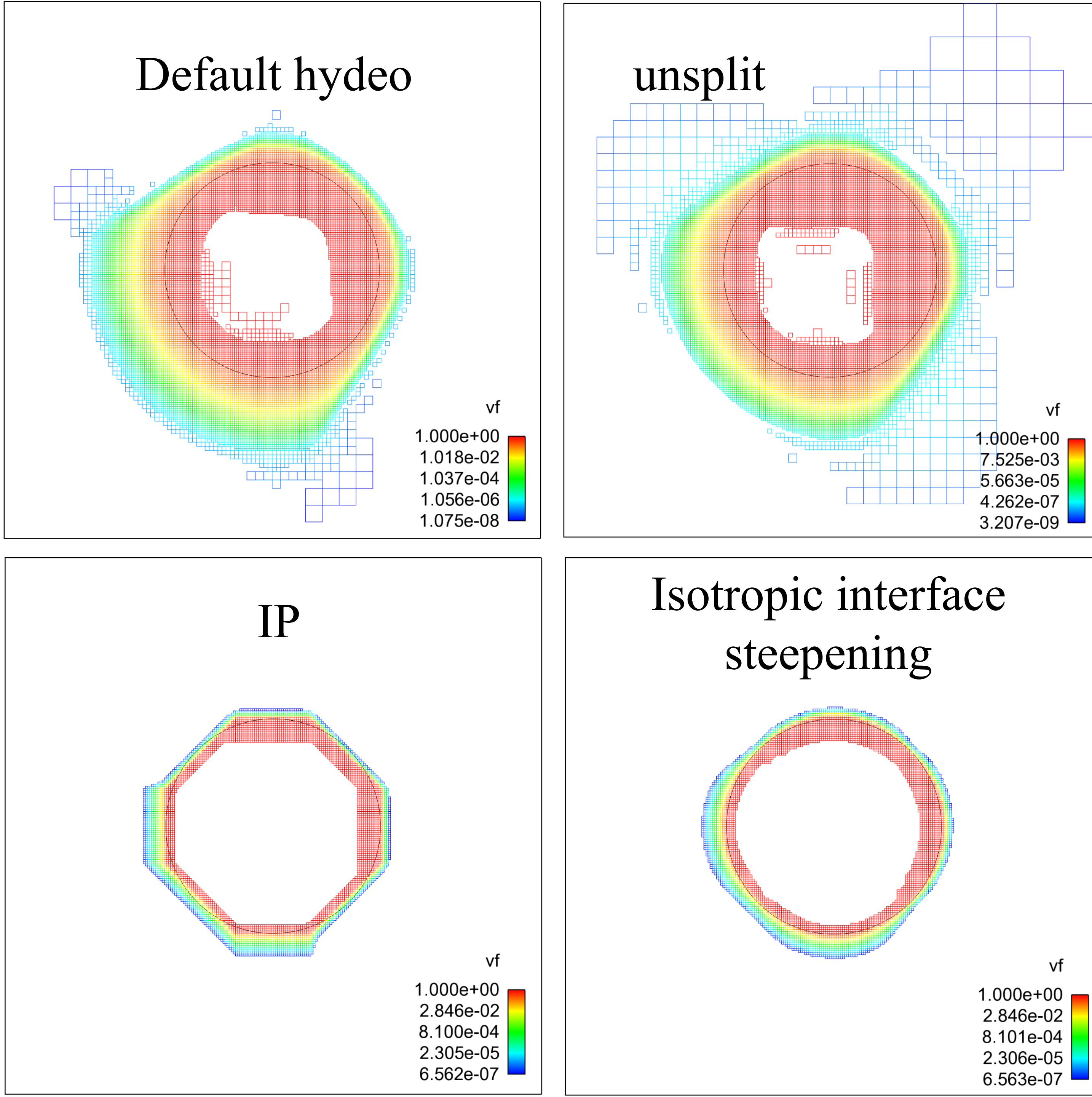
2D circular example : 2 materials and pressure balanced

Initially mixed cells are 1-cell wide.



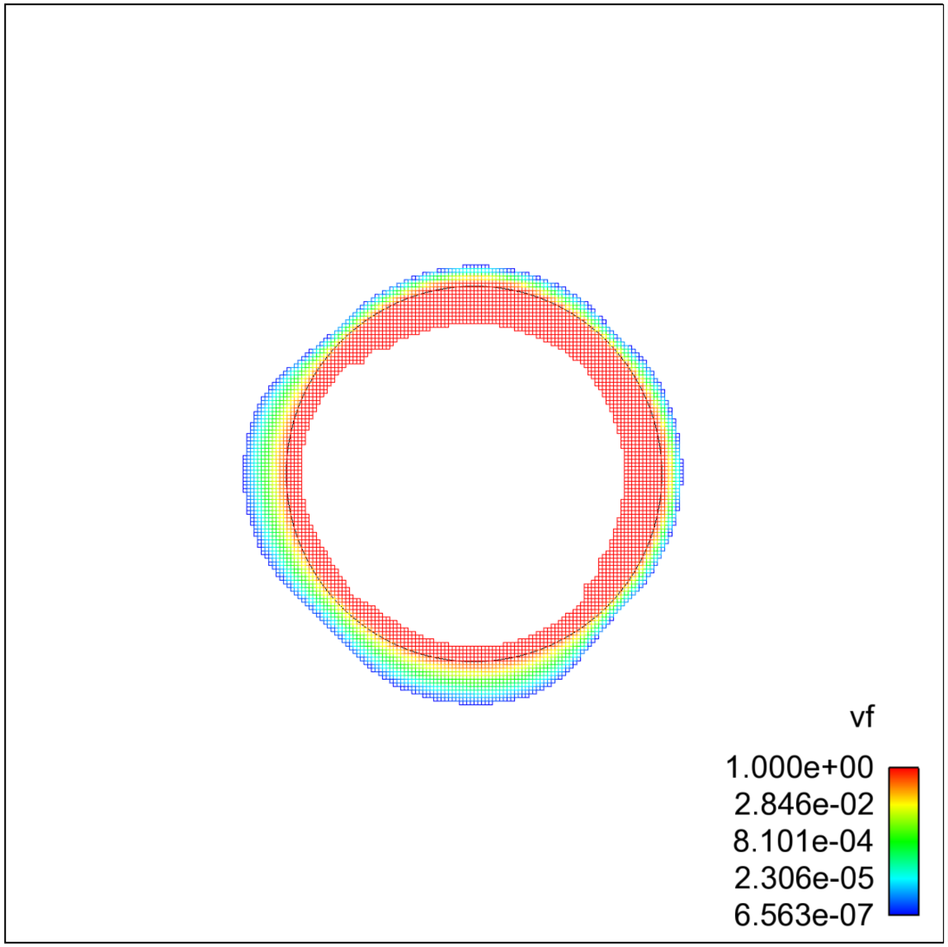
mixed cells

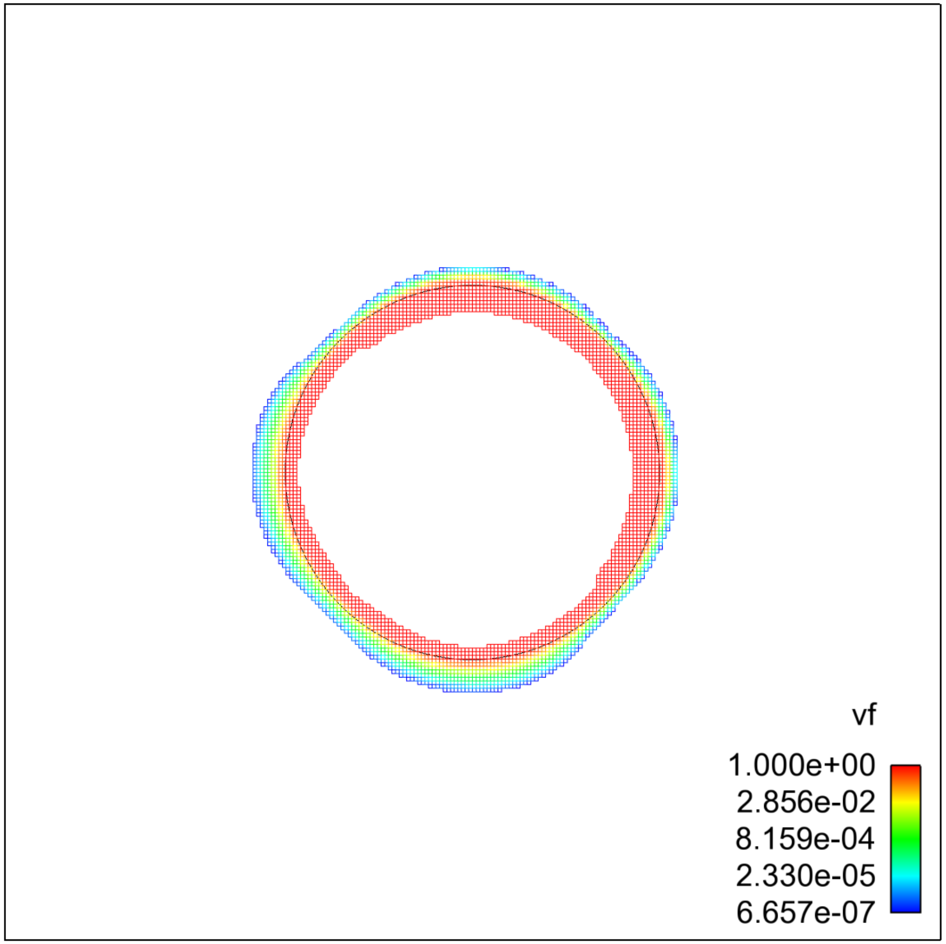
after 5 diagonal turns



Isotropic interface steepening

max interface steepening

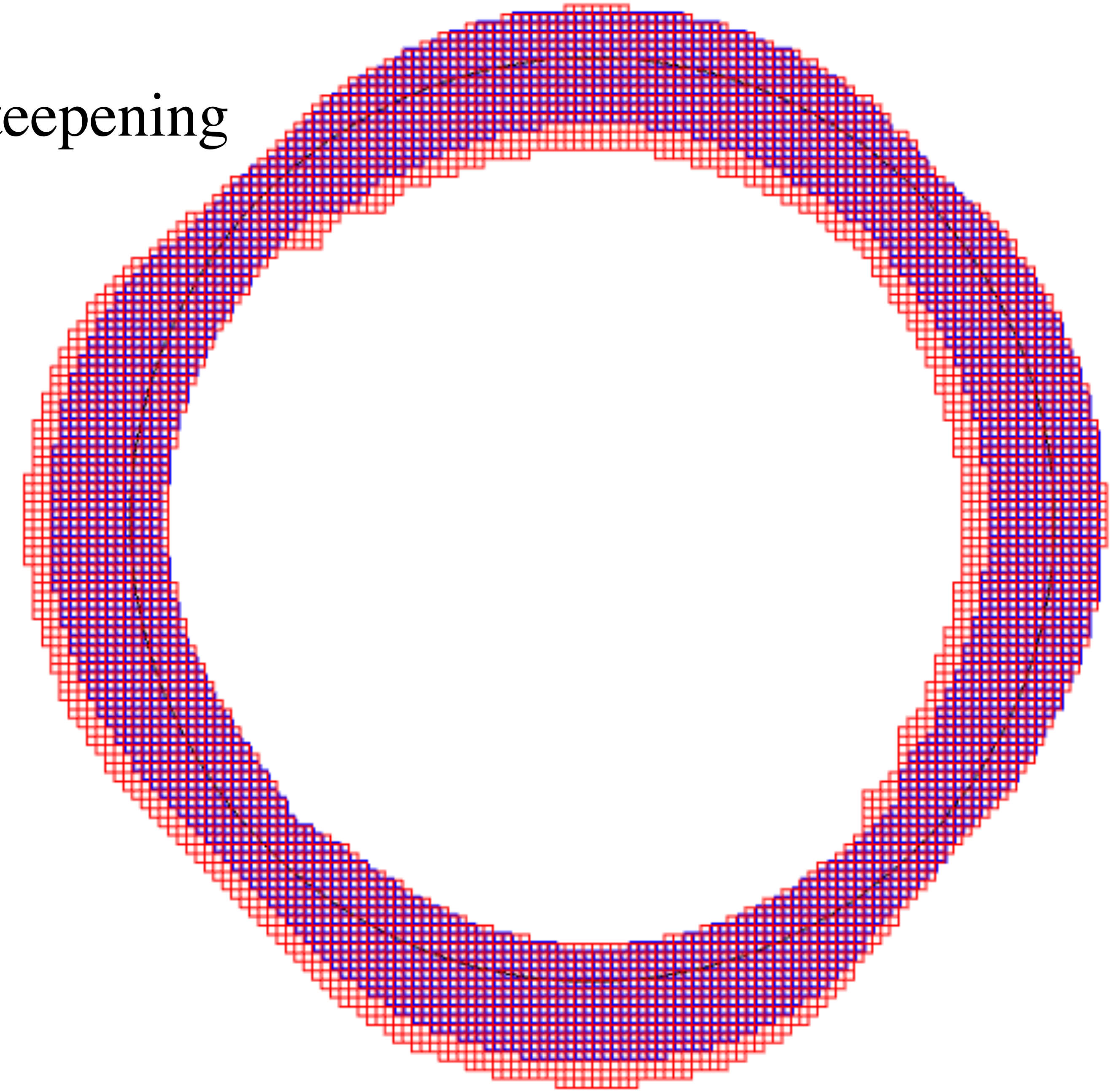




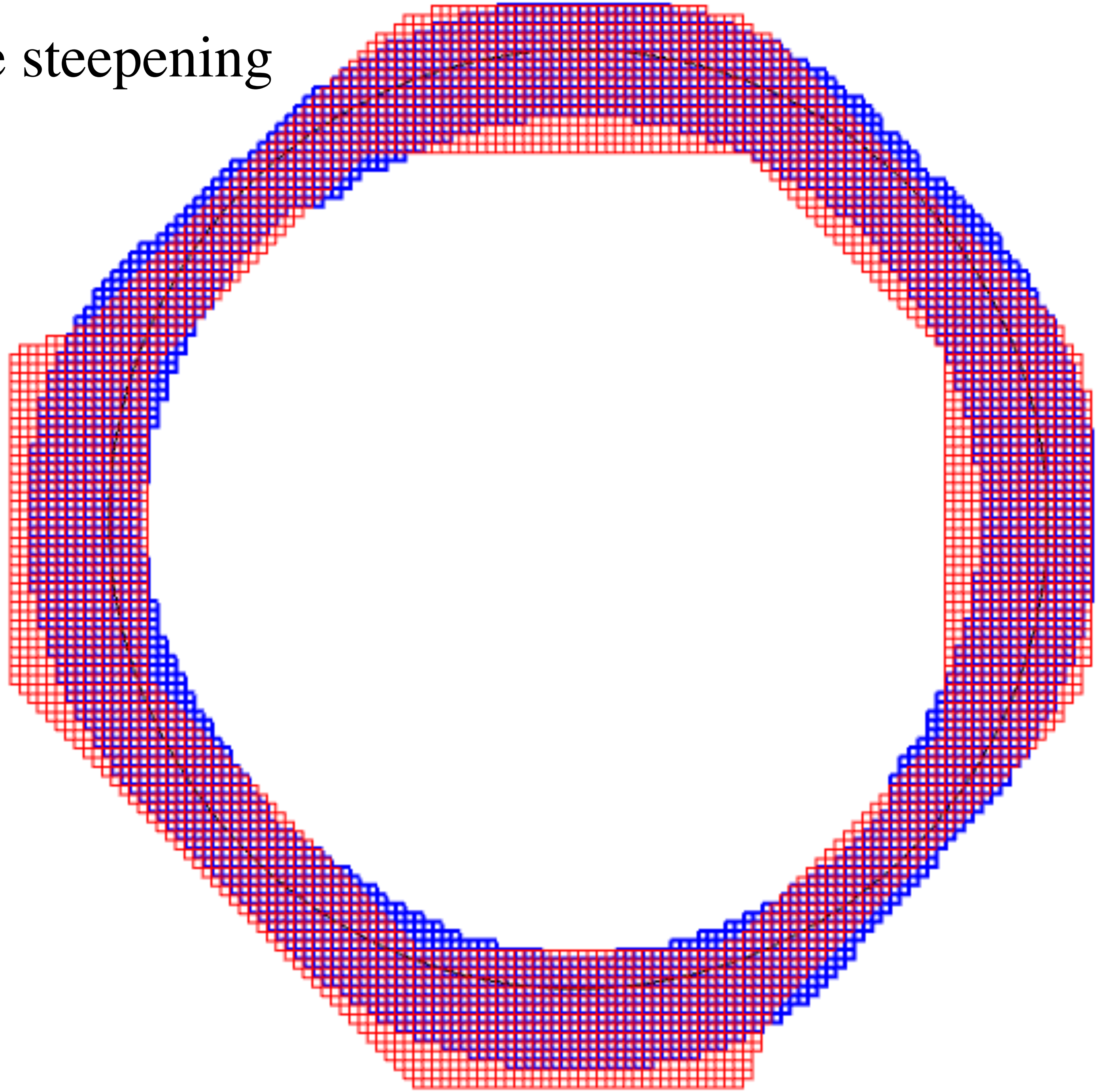
isotropic interface steepening

vs

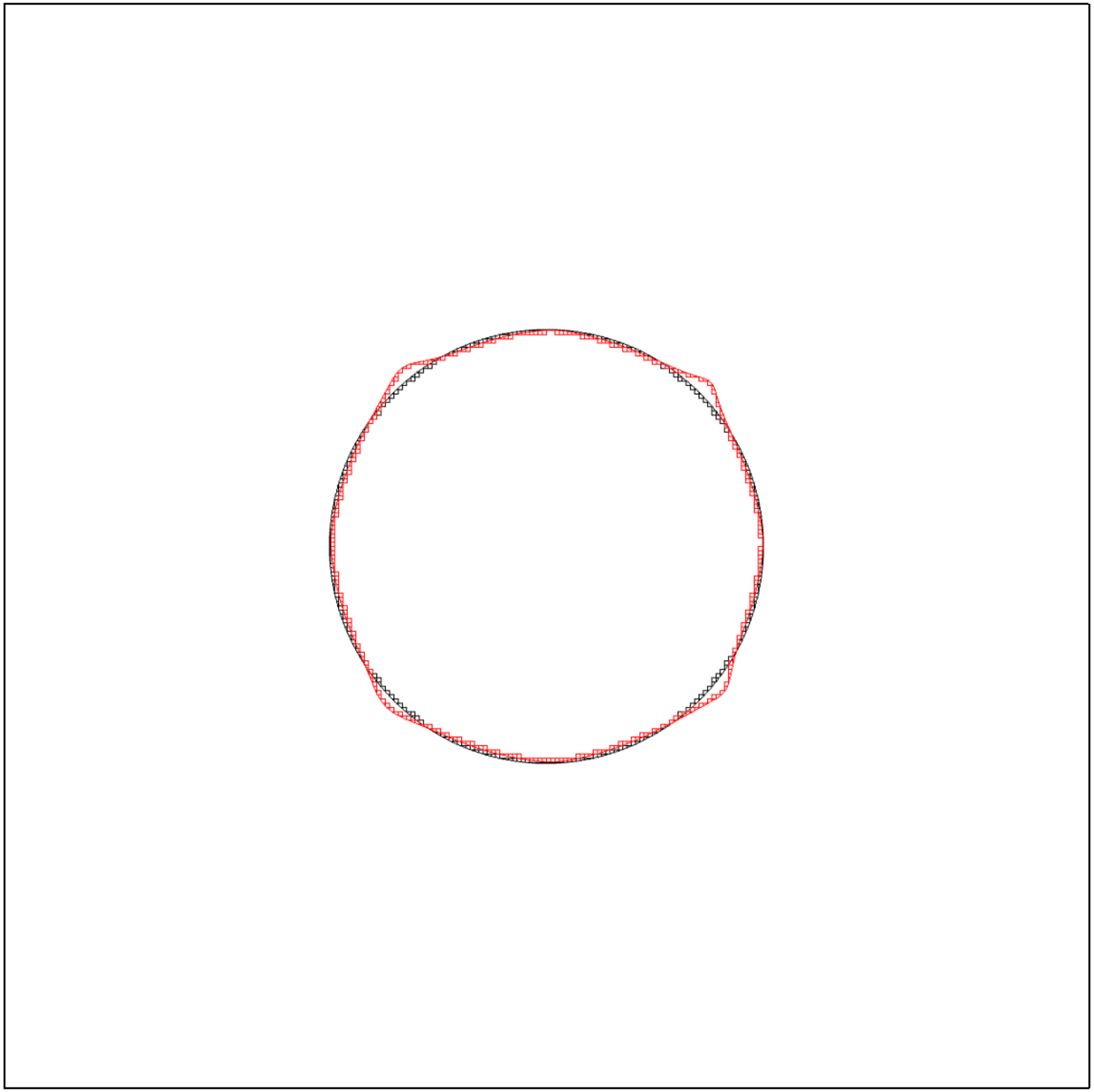
max interface steepening



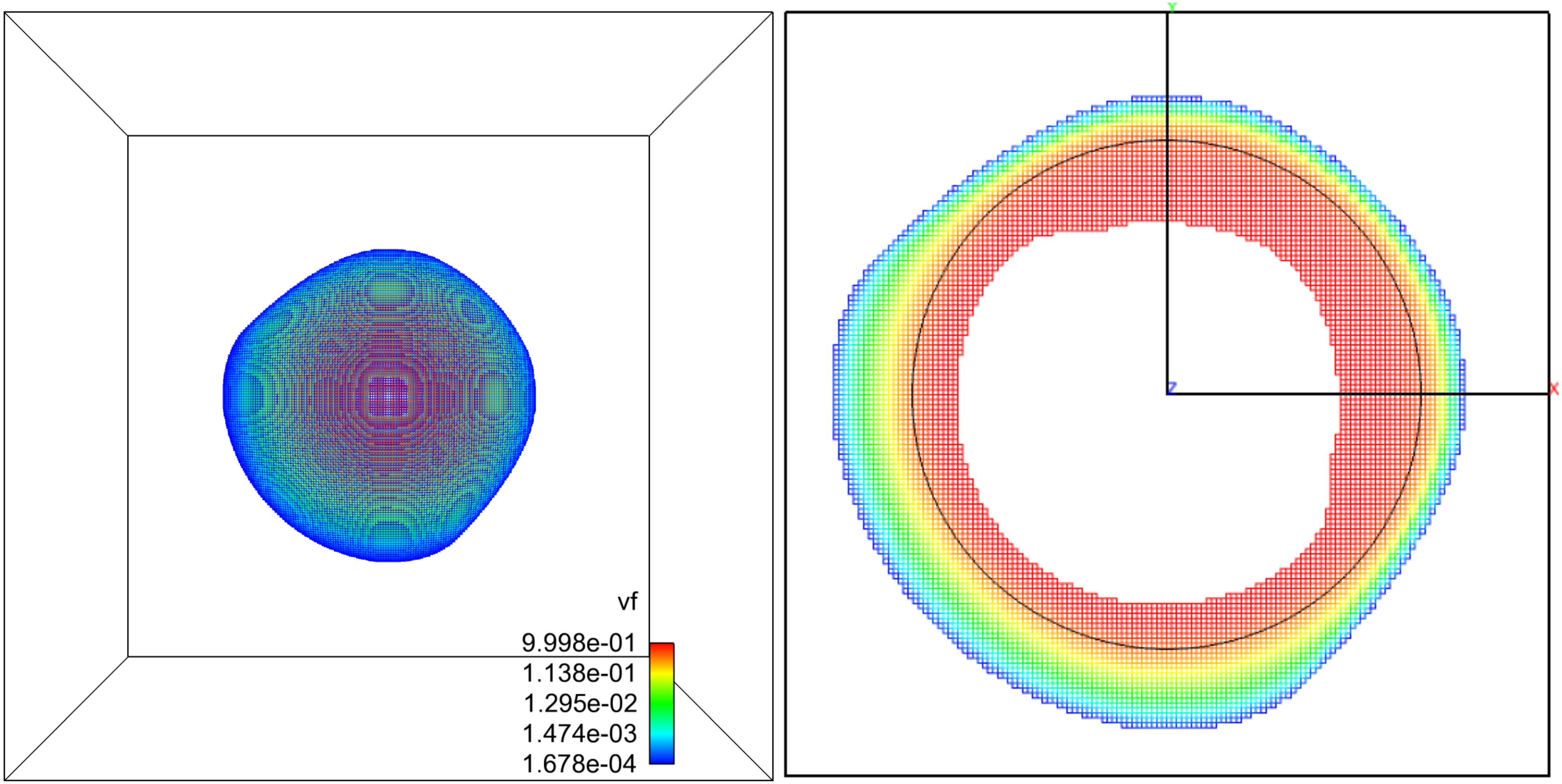
max interface steepening
vs
IP



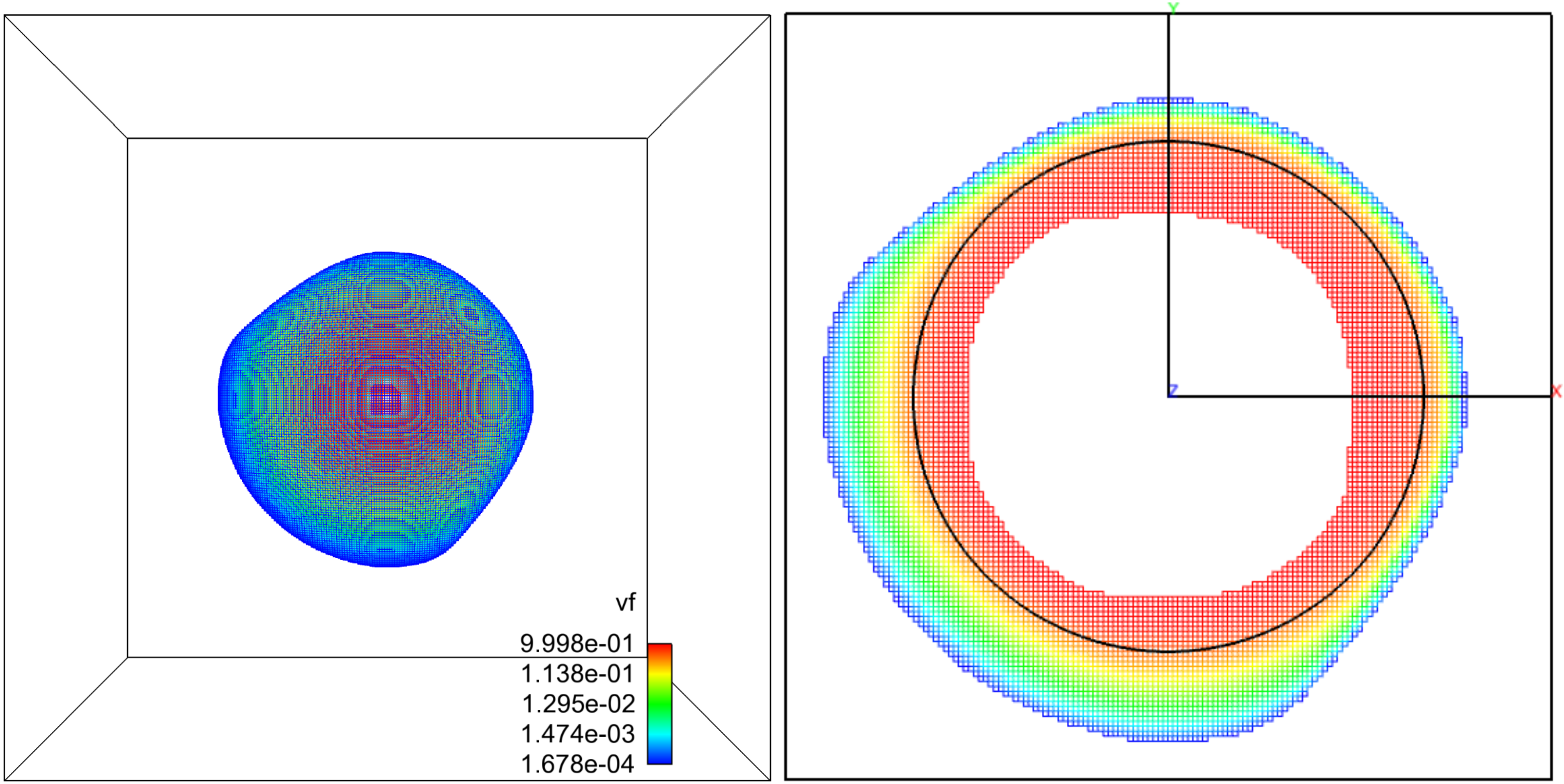
VoF



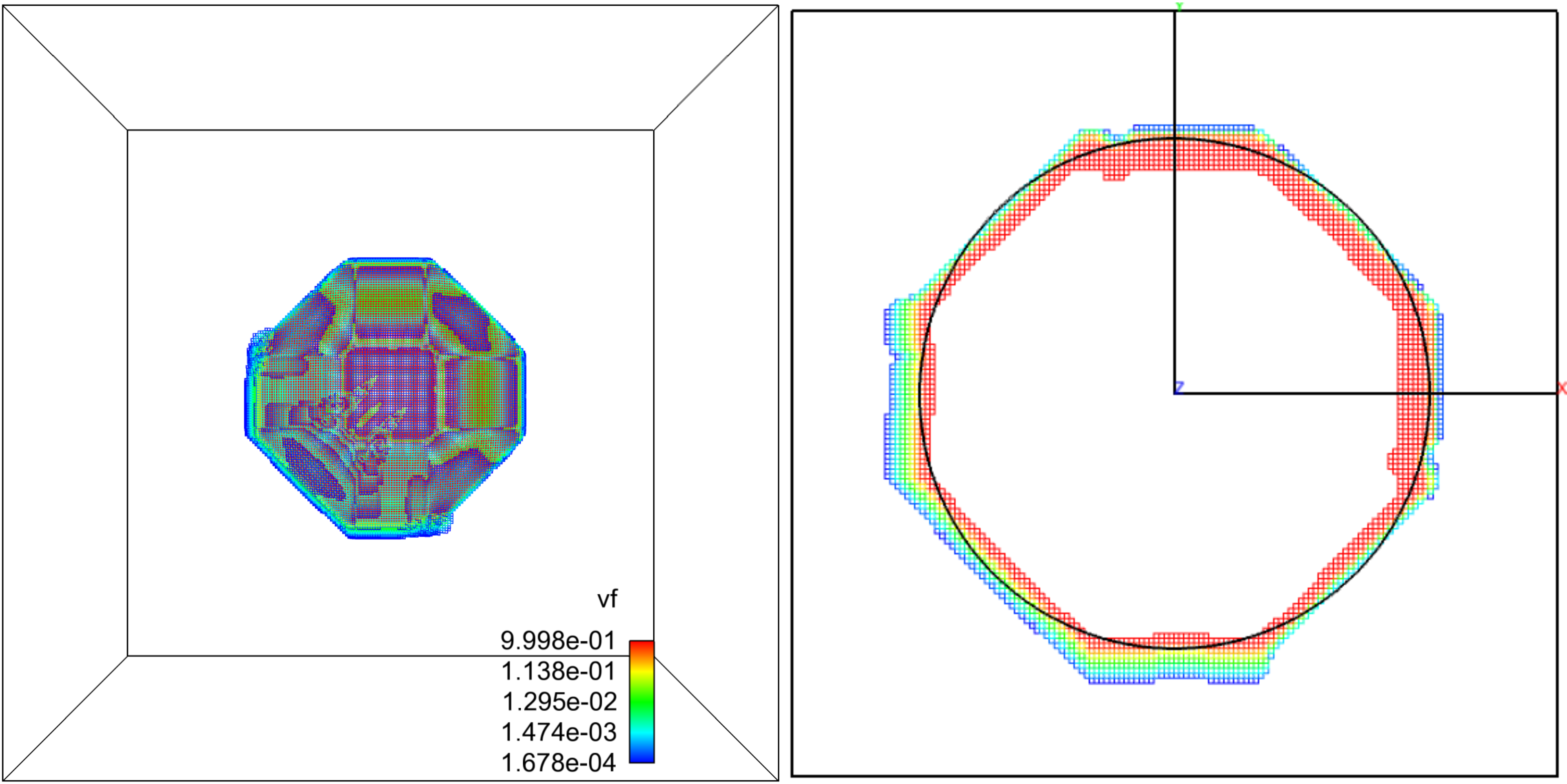
3D version: after 2 turns diagonally



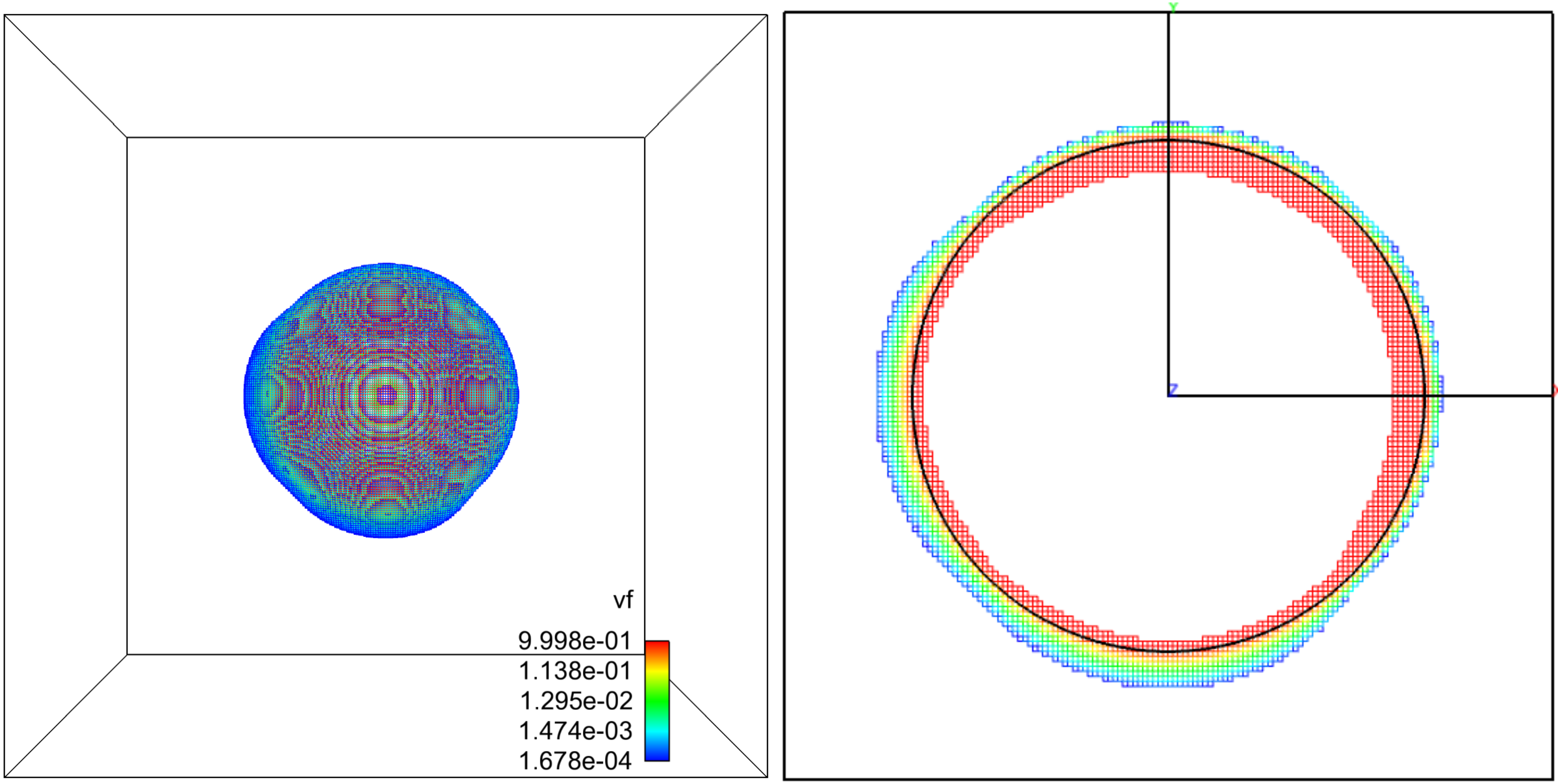
default hydro



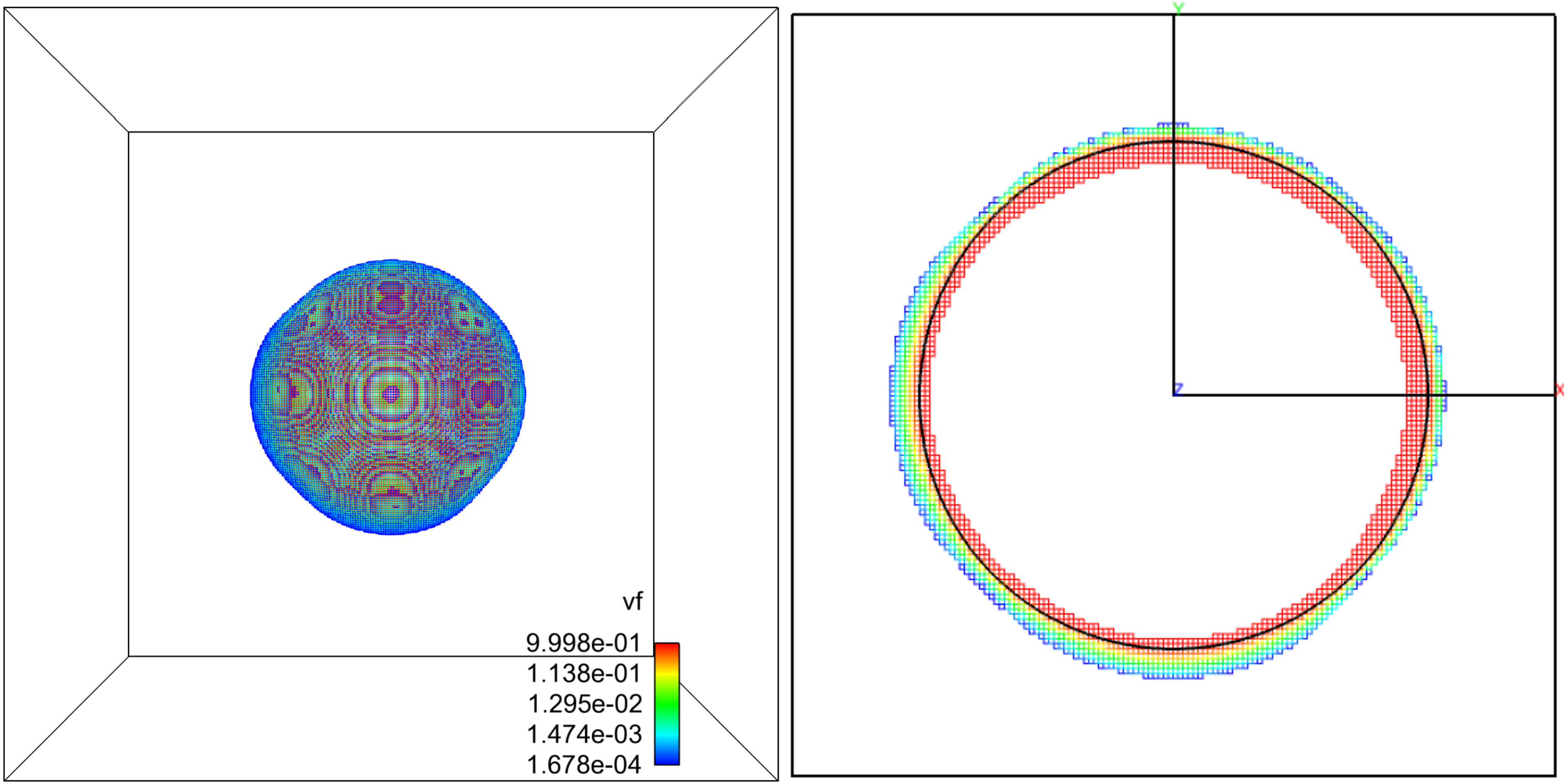
unsplit



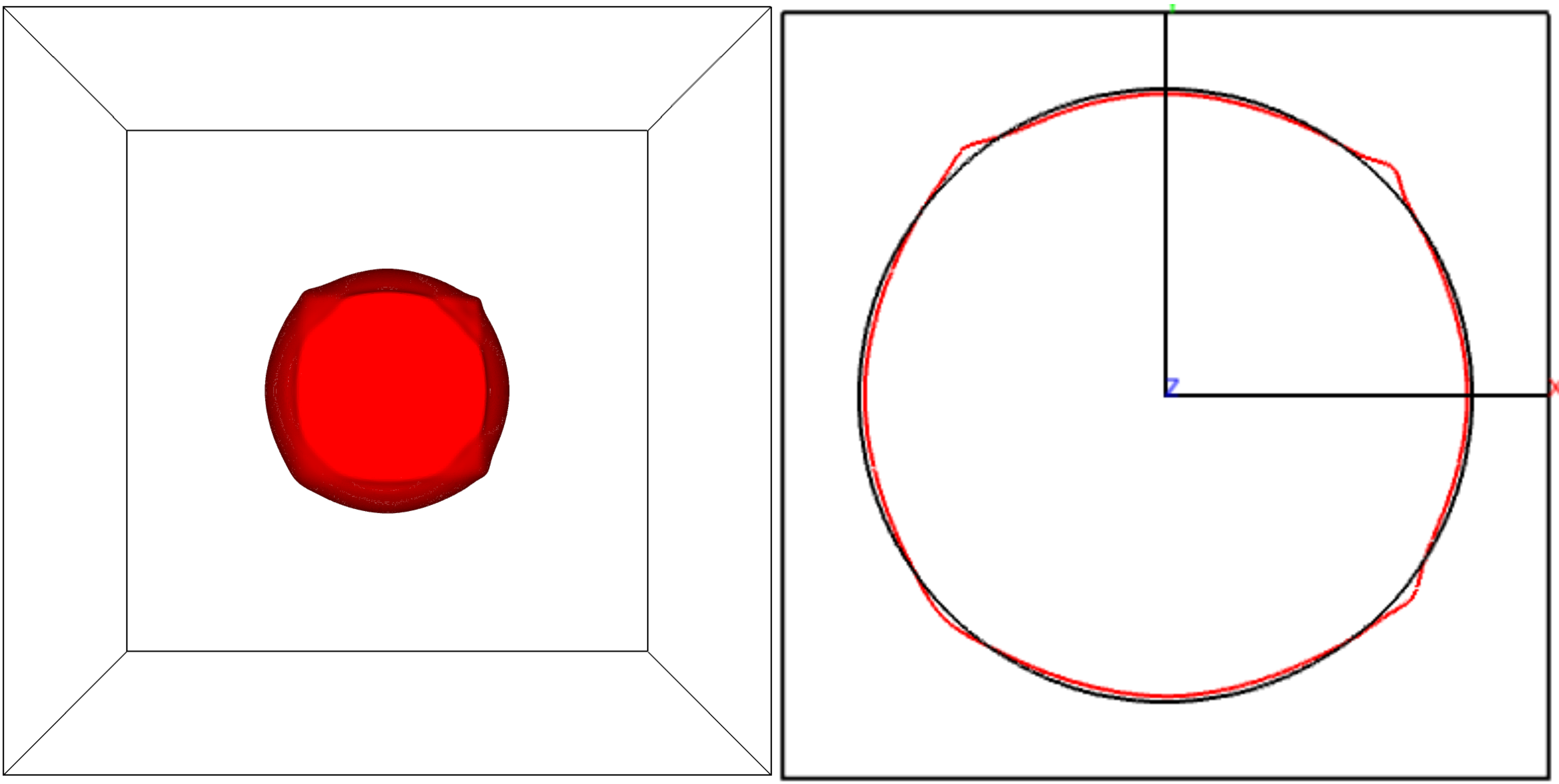
interface_option = 2



Isotropic interface steepening



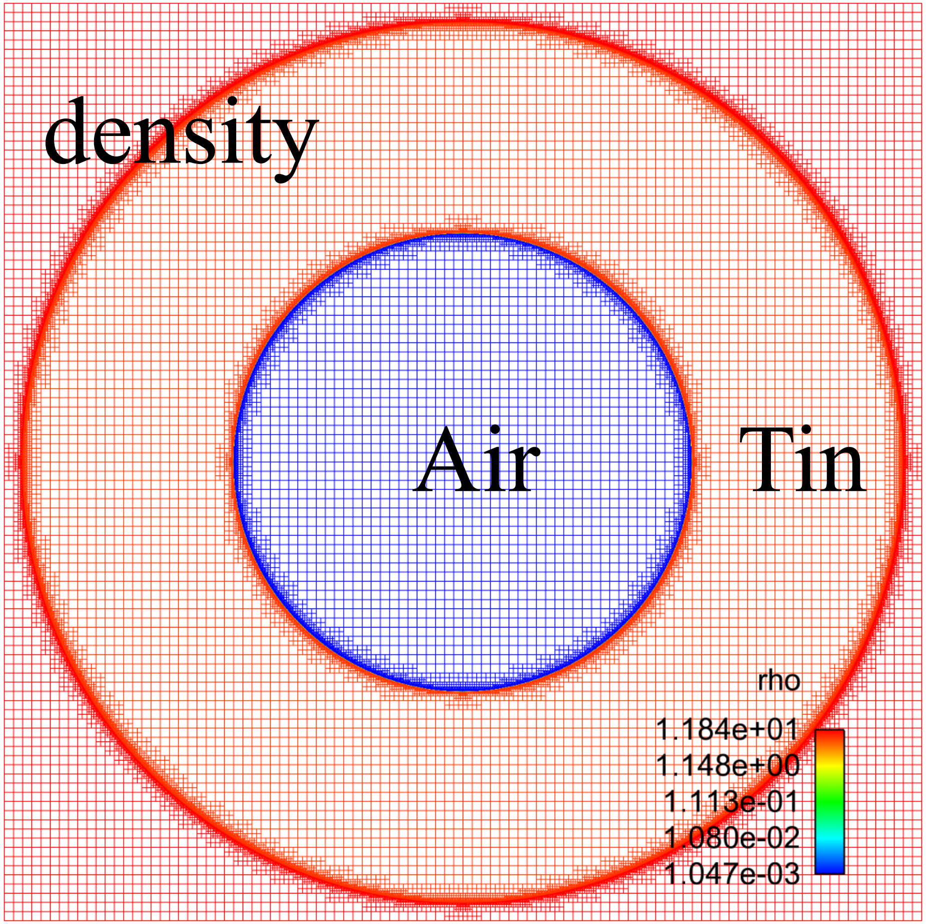
max_interface_steepening

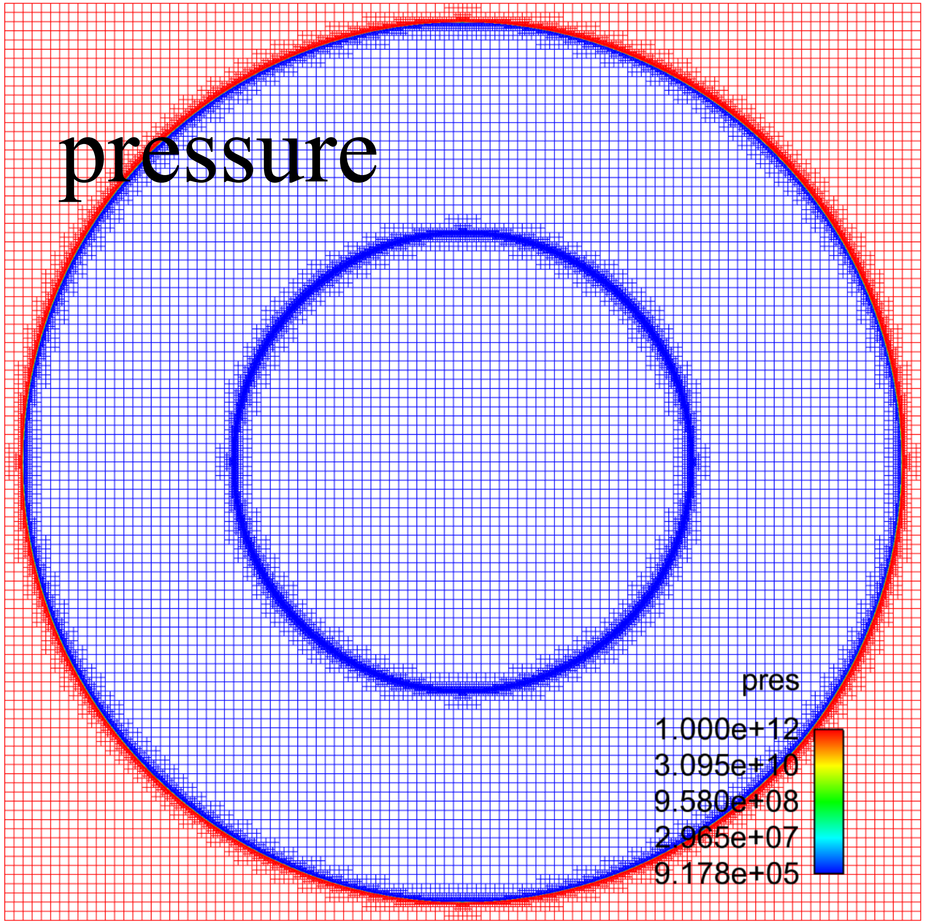


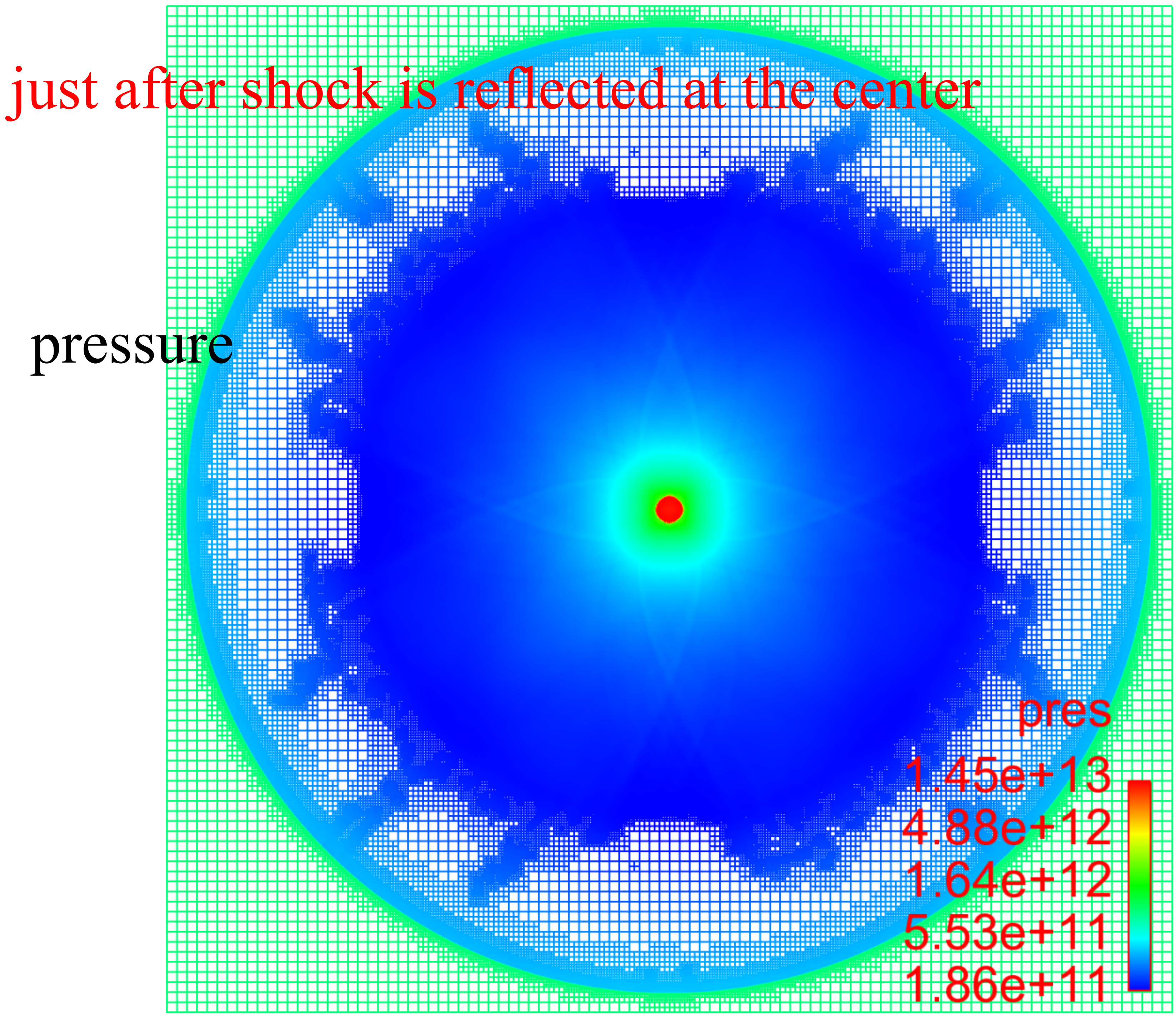
VoF

2D Implosion

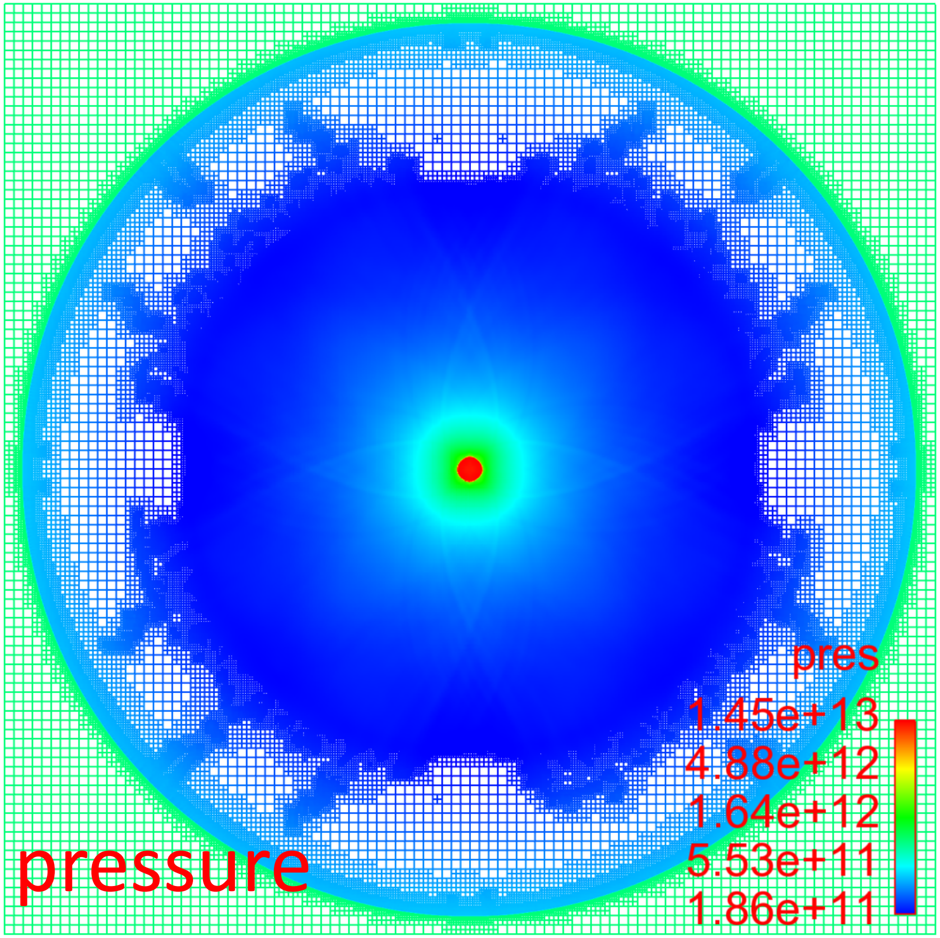
initial density and pressure of two materials



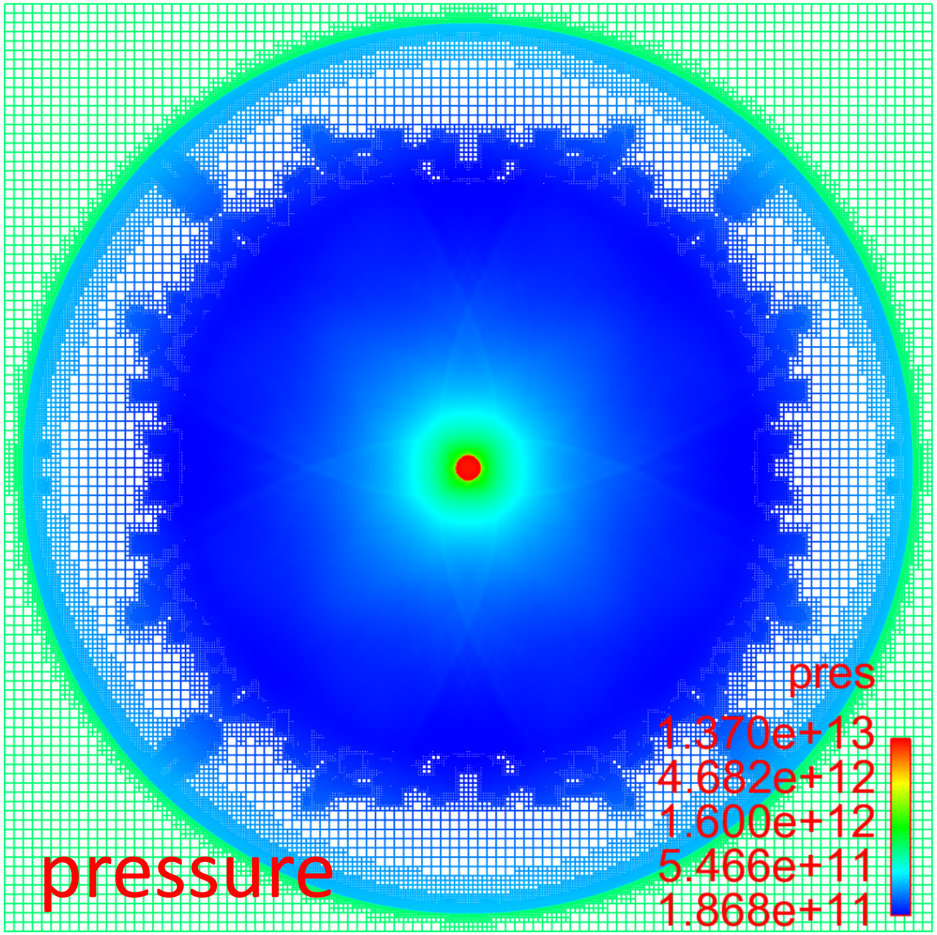



just after shock is reflected at the center
pressure
pres
1.45e+13
4.88e+12
1.64e+12
5.53e+11
1.86e+11

VoF



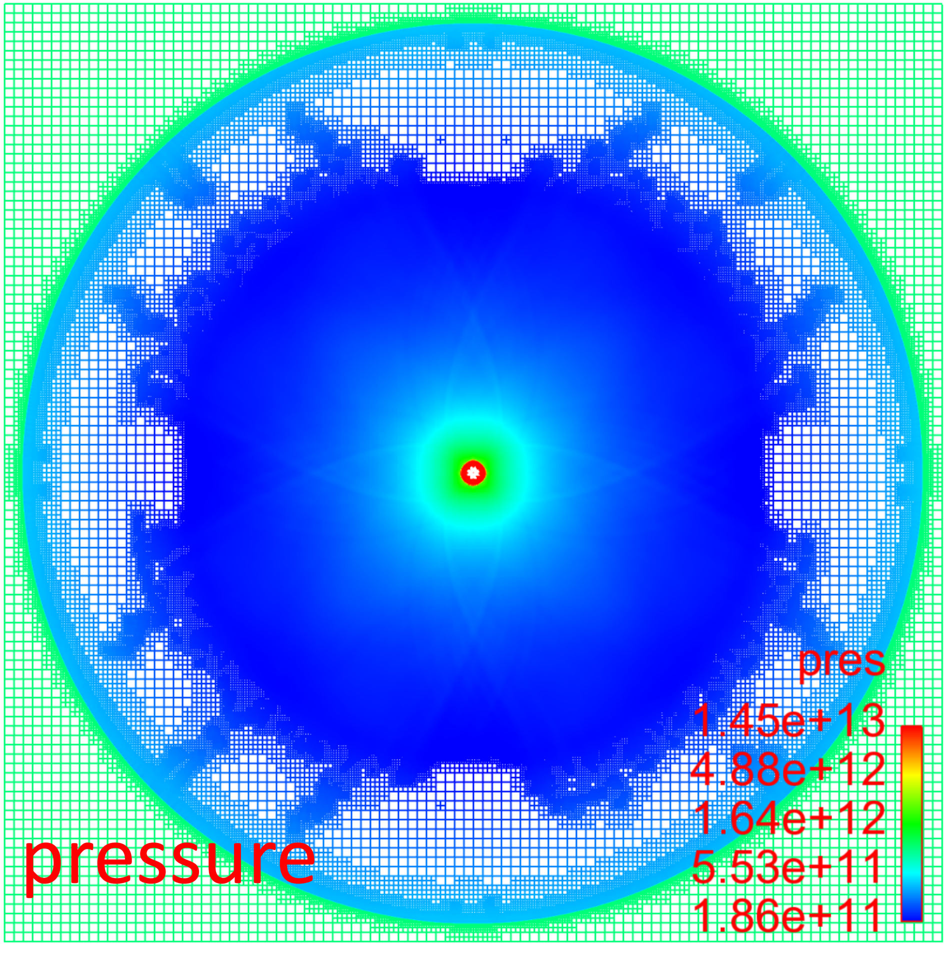
default hydro



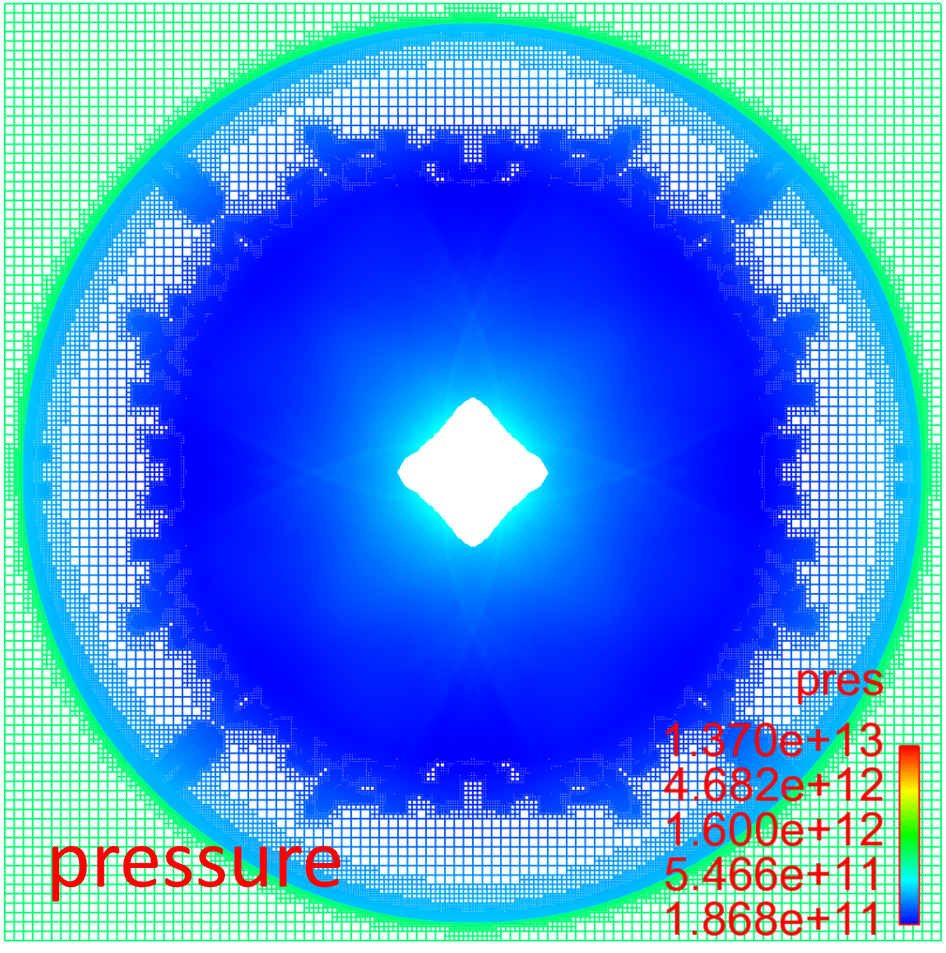
just after shock is reflected at the center

mixed cells excluded

VoF



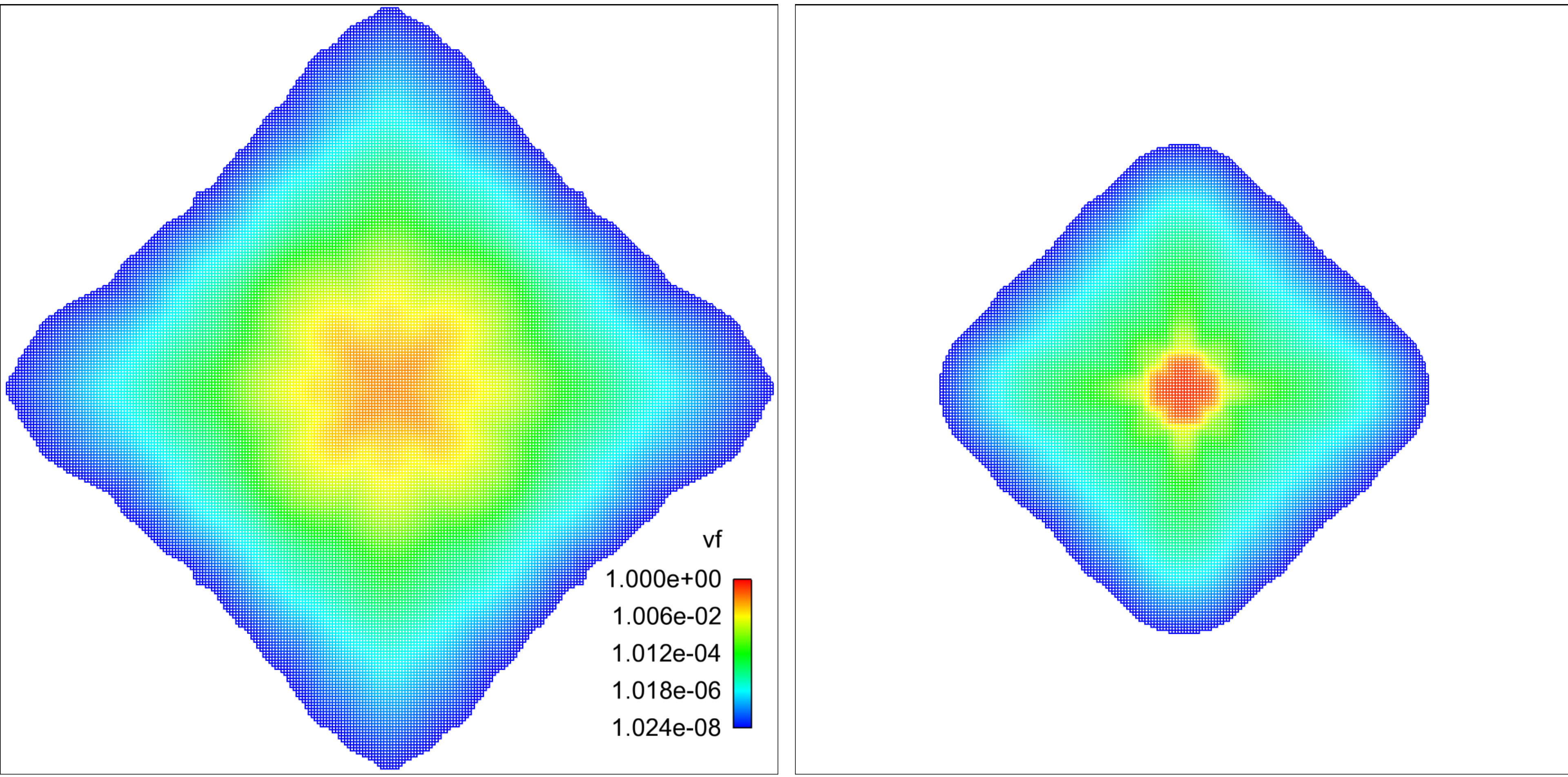
default hydro



volume fraction of air on mixed cells

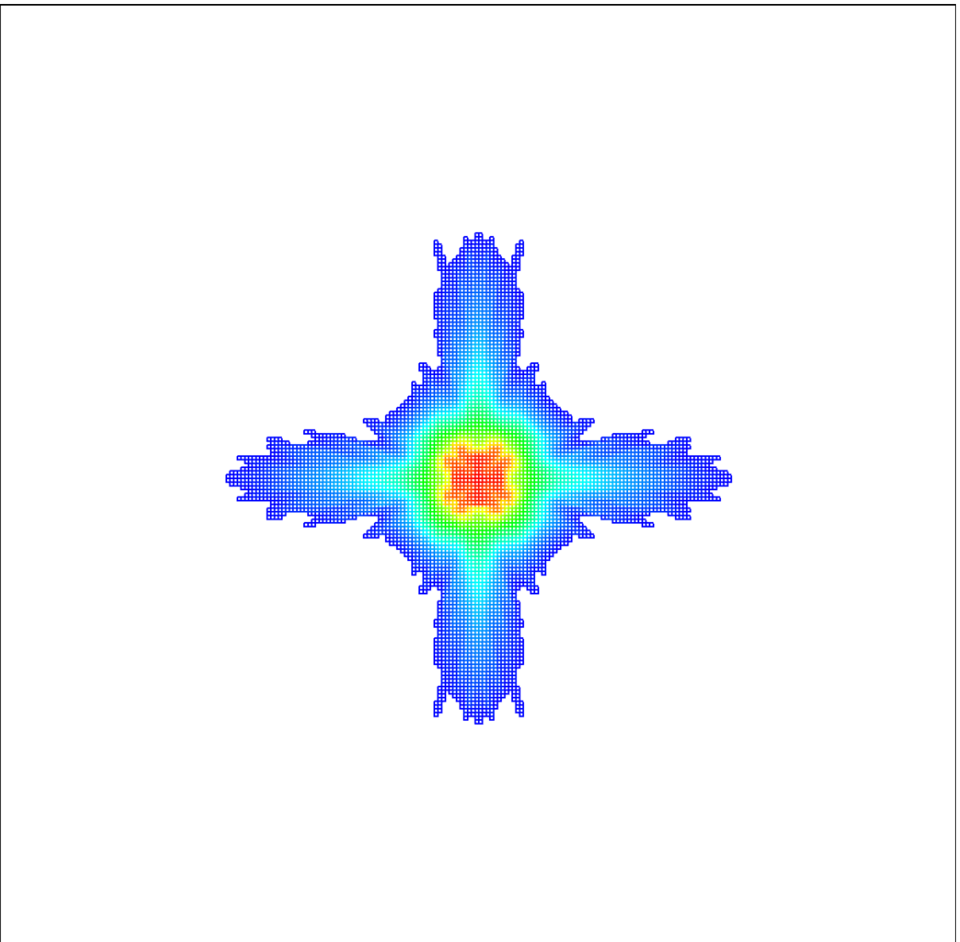
default hydro

unsplit hydro

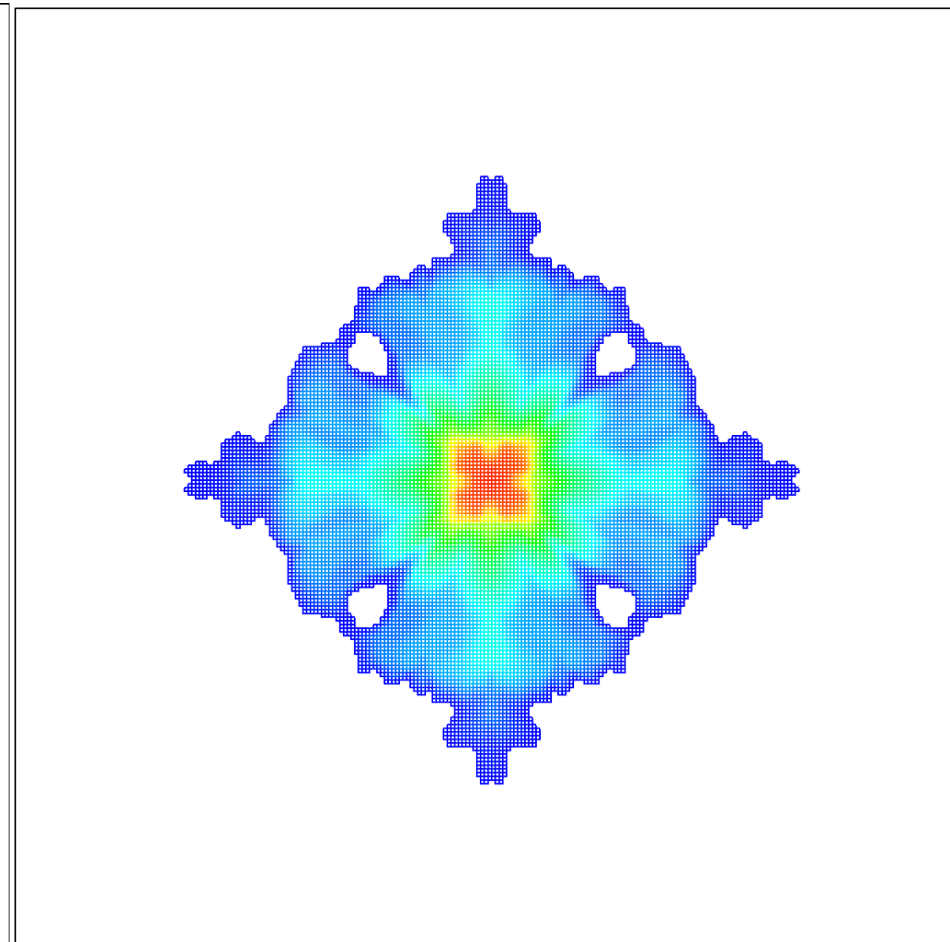


volume fraction of air on mixed cells

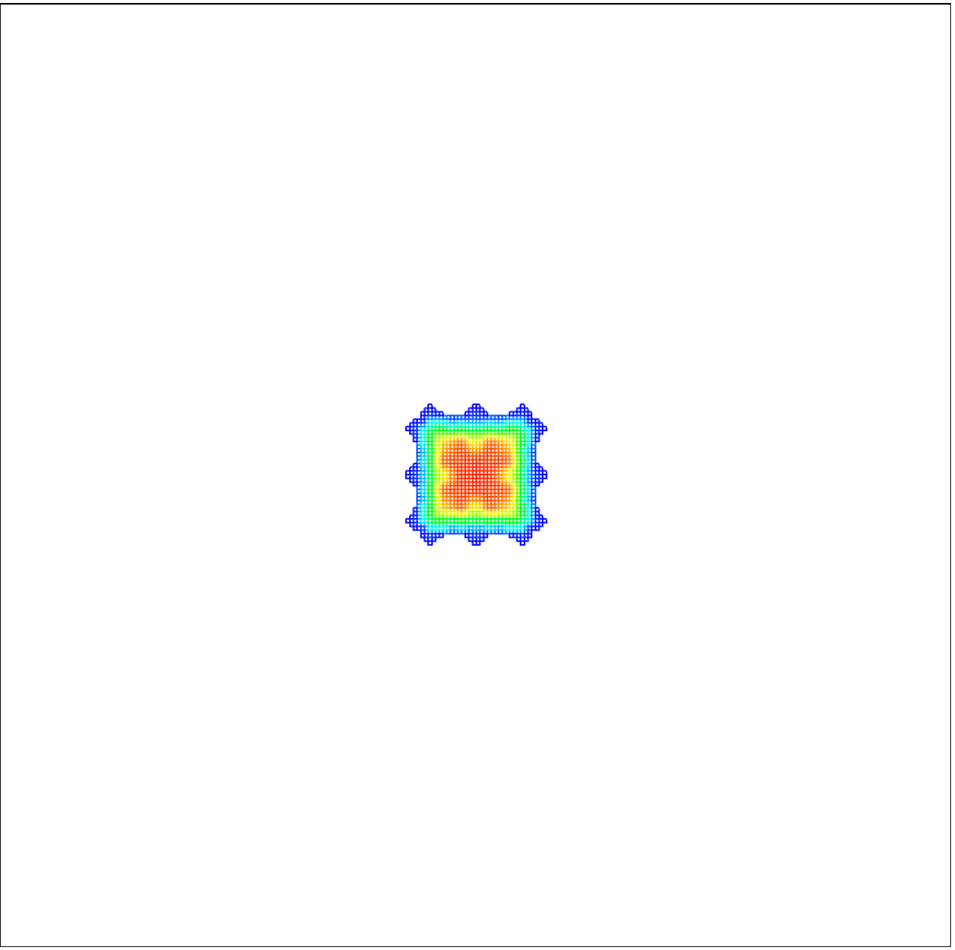
IP



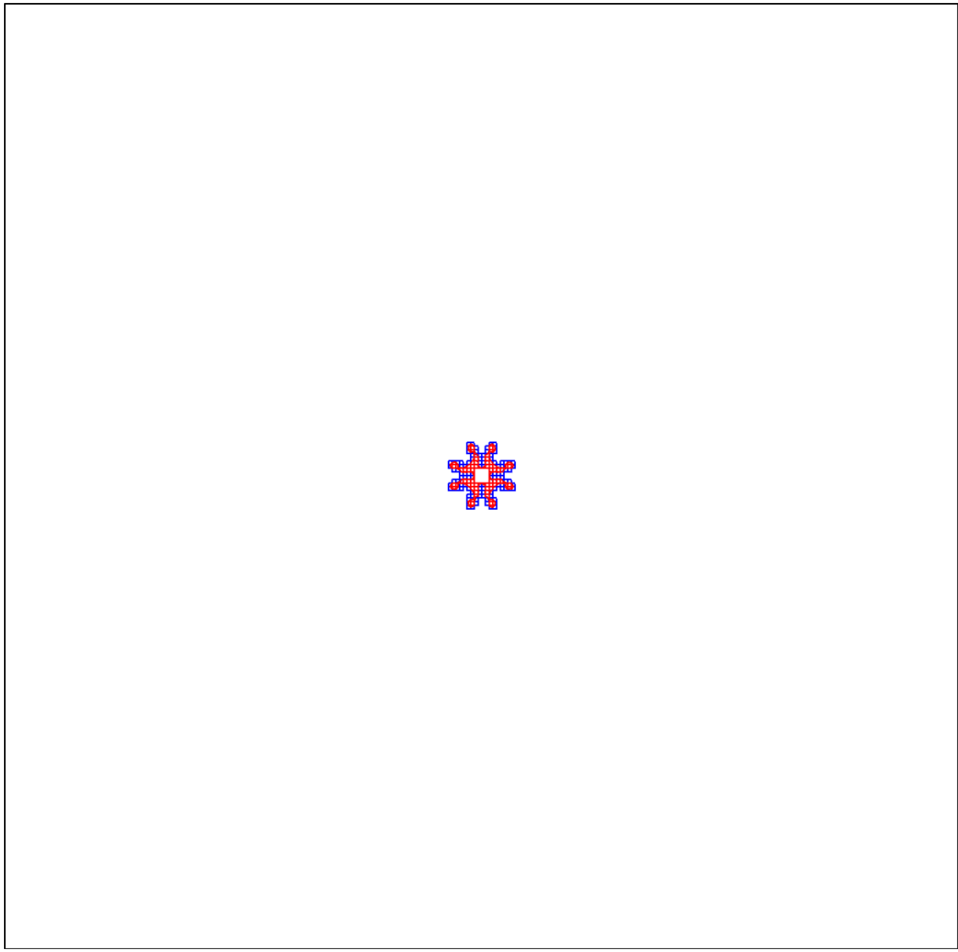
isotropic interface steepening



max interface steepening

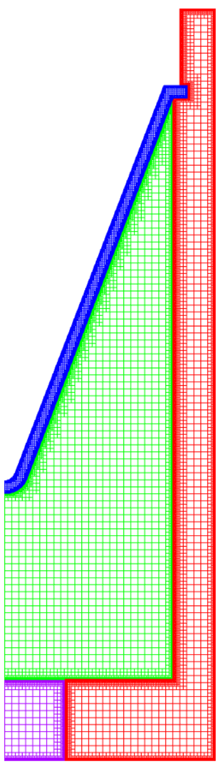


VoF



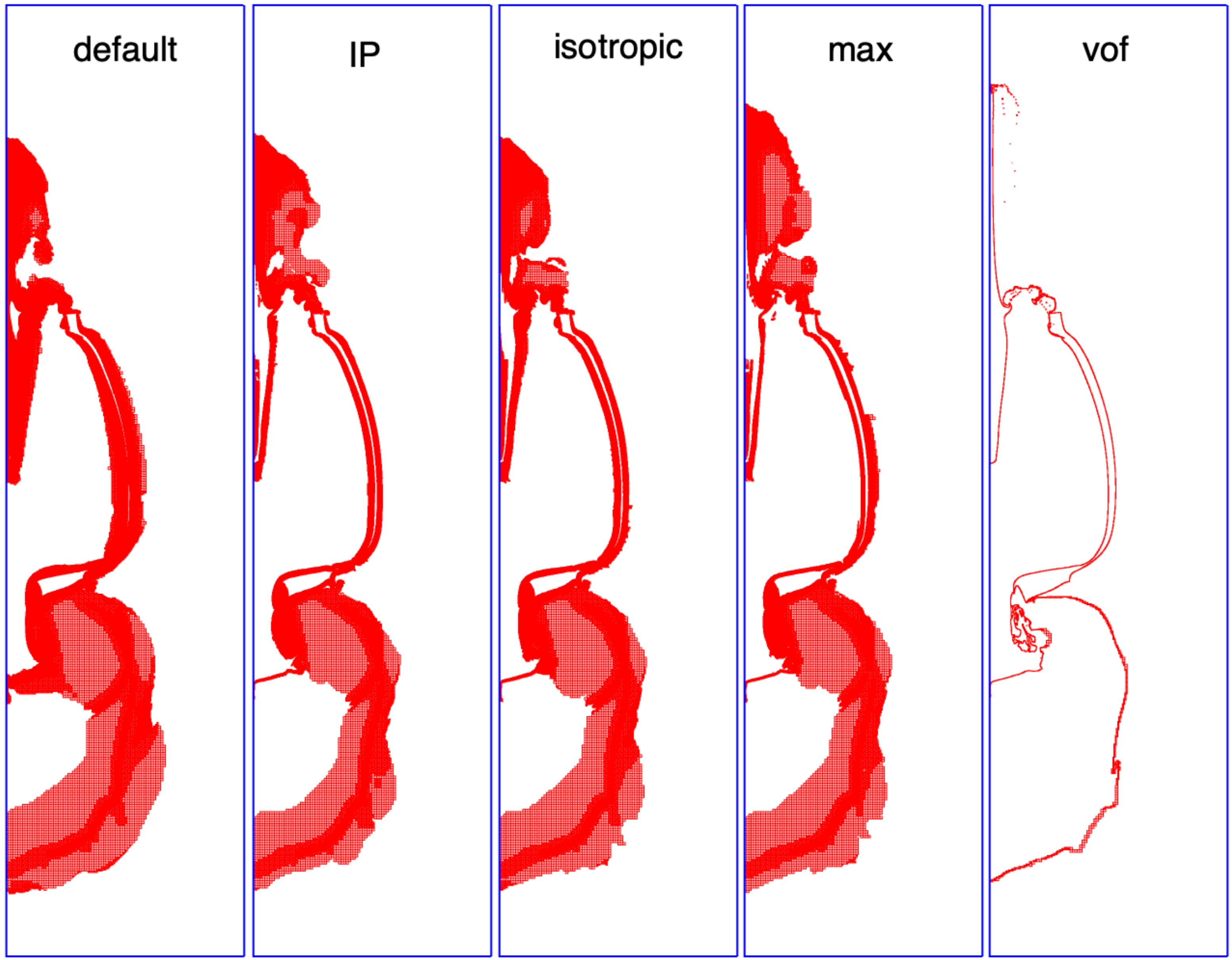
Shaped Charge

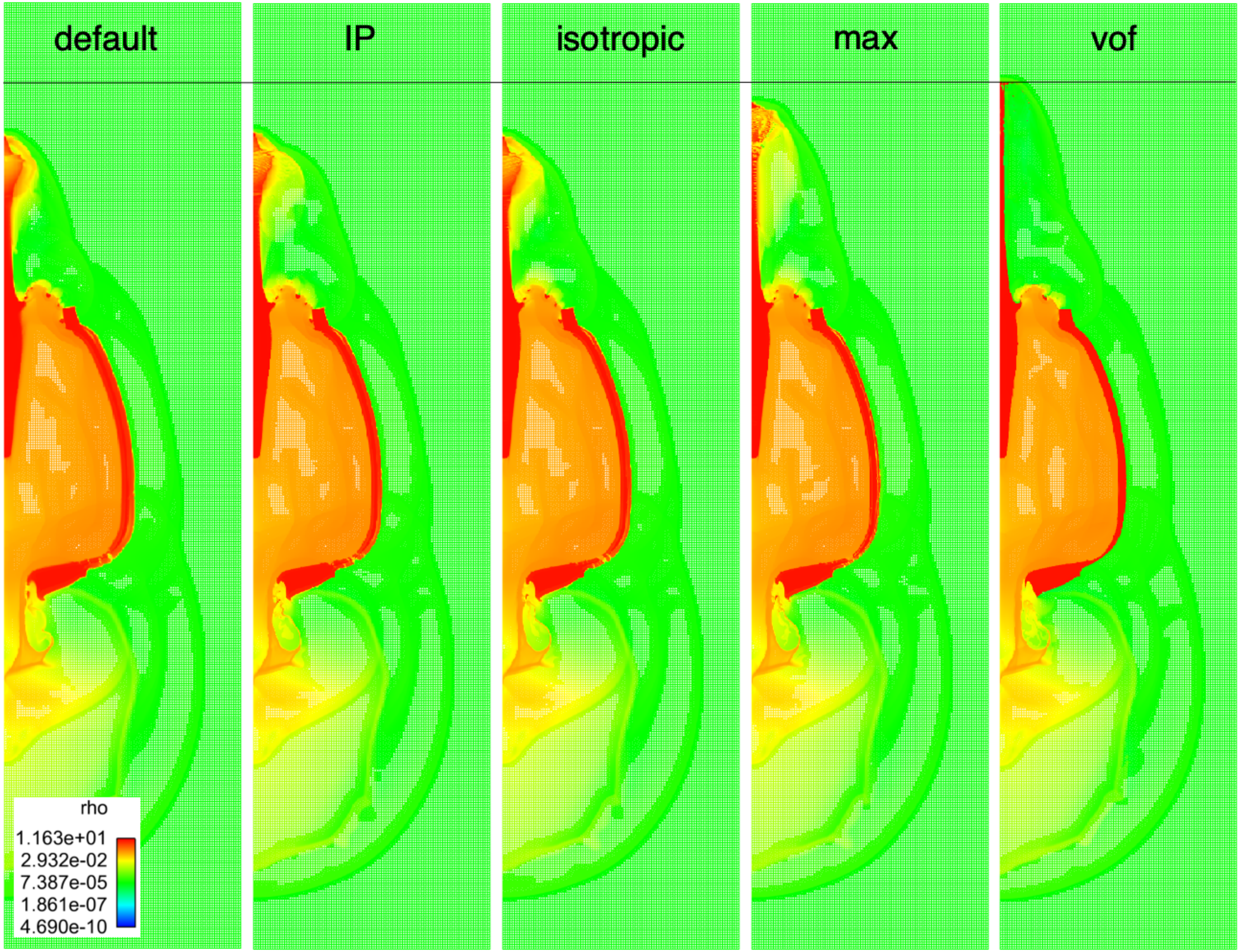
simulation domain



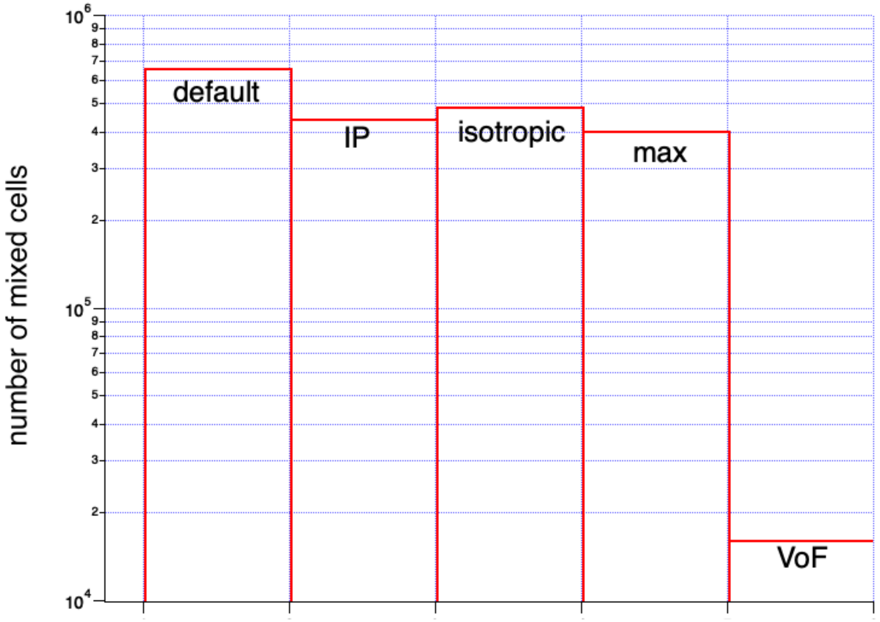
materials

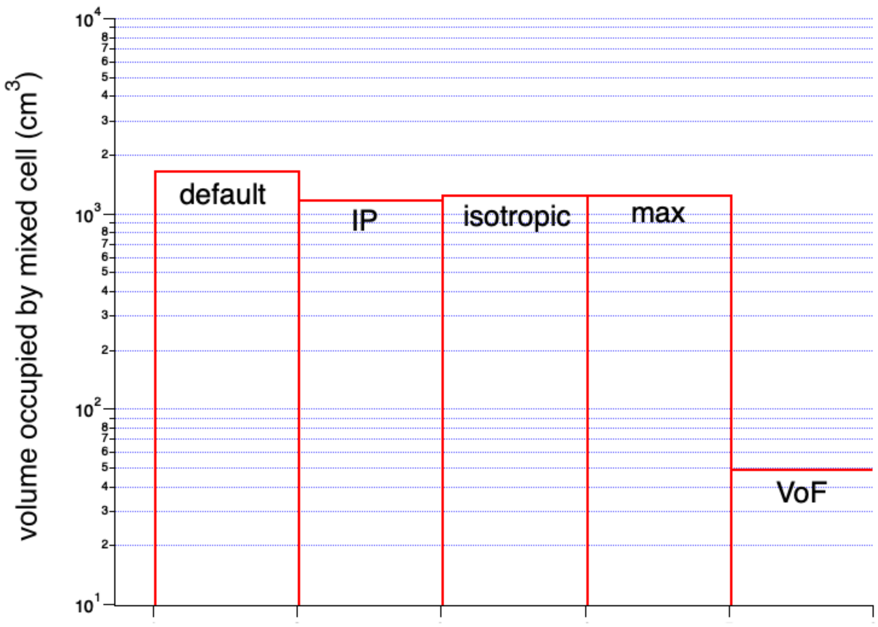
mixed cells from 5 hydro options




default
IP
isotropic
max
vof
rho
1.163e+01
2.932e-02
7.387e-05
1.861e-07
4.690e-10

Number of mixed cells and volume occupied by mixed cells





Conclusions

- Split & unsplit hydro without interface treatment are diffusive for material, and an interface could be spread over about 40 cells.
- Increase of AMR level reduces the numerical mixing (in space), but not by a factor 2 for each level.
- Standard interface steepening (IP) could reduce numerical mixing by a factor 2 in number of mixed cells, and more than a factor 2 spatially.
- The option, isotropic interface steepening, keeps isotropic feature well, but introduces a little more numerical mixing than IP.
- The option, max_interface_steepening, introduces less numerical mixing compared with IP and isotropic interface steepening, and also keeps isotropic feature well.
- If applicable, VoF could reduce numerical mixing to minimum within the framework of Eulerian calculations.
- Higher order methods don't necessarily indicate less numerical mixing. A higher order method could introduce more numerical mixing than a lower order one.